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Assessment of Fatigue Crack Growth Rate Based on Physics-Informed Neural Networks in Hydrogen Environments

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Abstract. The safety of hydrogen storage and transportation systems is a fundamental component of clean energy, so the fatigue performance of metallic materials is very important. Nevertheless, the hydrogen embrittling effect caused by hydrogen environments mostly increases the rate at which fatigue cracks grow in the materials, and therefore, the problem of predicting material lifespan drastically increases. Conventional fatigue life prediction techniques make use of experimental tests and numerical modelling, but are hindered by high data collection costs and the complexity of modelling multi-physics coupled behaviour. Over the past several years, a new solution has been developed, Physics-Informed Neural Networks (PINNs), to serve fatigue crack prediction in hydrogen environments, capitalizing on their strengths of combining physical laws with data-driven methods. PINNs have more advanced capacities in cross-scale modelling and improved the reputation of model forecasts, which outperforms the traditional approach with high precision and efficiency in safe hydrogen energy infrastructure design.

Keywords: fatigue crack growth rate, Physics-Informed Neural Networks, fatigue life predictions.

1. Overview of Physics-Informed Neural Networks

Physics-Informed Neural Networks (PINNs) are a type of machine learning model

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[1] [2] that combines deep learning and physics, whose key goal is to amplify the generalization behavior of the model at low data regimes, or at noisy environments, by enforcing physical laws as prior knowledge in the neural network [3]. Unlike traditional model-driven methods, PINNs enforce (physical) constraints (such as partial differential equations) and (physical) boundary conditions) on the output of the learned network in the loss function and thus ensure that the computed solutions are physically reasonable [4]. PINNs can be used to integrate physical information by considering governing equations (i.e., the Navier-Stokes equations) as contributions to the loss. Further interactivity of PINNs has also been improved with the introduction of adaptive activation functions and residual integrators. Advances in adaptive regulations and hardware enablement technologies [5] have implied that PINNs are increasingly becoming one of the instruments of the fundamentals of the entirety frameworks.

Hydrogen embrittlement leads to local stress concentration [6] that causes formation and propagation of cracks in steel structures, increasing by one or multiple orders of magnitude the Fatigue Crack Growth Rate (FCGR) and thereby potentially causing brittle fracture. That poses a major threat to the hydrogen pipeline material, such as the pipeline steel. Therefore, to determine the damage tolerance and fatigue failure of hydrogen energy equipment, it is significant to effectively and precisely forecast the FCGR to design [7] [8]. With the introduction of machine learning methods, a new avenue of study on the subject is possible because the strong nonlinear processing and multivariate learning of machine learning could yield accurate measurements of FCGR. However, traditional machine-learning methods [9] require large amounts of quality test data [10], and Fatigue Crack Growth (FCG) hydrogen test studies are costly and could lead to an inability to generalize the models, as well as to physical inconsistency of the result. So if hydrogen-induced FCG models are implemented into the PINN system, it is possible to exploit the abilities of the model; it requires less information, yet it promotes the derivation of intricate nonlinear issues, enhancing the precision and effectiveness of finding the crack growth rate.

2. Hydrogen-Induced fatigue crack growth model

2.1. Fatigue Crack Growth model

A critical realisation and investigation of the processes of Hydrogen-Assisted Fatigue Crack Growth (HA-FCG) could help in the development of a broad model founded on the physics of material deformation. The metallic materials fatigue damage behavior [11] and crack growth behavior in hydrogen environments [12] have qualitatively different characteristics than the same behavior in more traditional environments. Hydrogen atoms would enter the material, resulting in loss of mechanical properties [13] and, consequently, causing rapid initiation and propagation of fatigue cracks [14]. Thus, the development of a proper model of hydrogen-induced FCG is especially valuable both to learn more about this damage degradation phenomenon and to provide recommendations on successful engineering outcomes.

The damage caused by hydrogen-induced fatigue is usually classified into three types: hydrogen-enhanced decohesion, hydrogen-enhanced local plasticity, and adsorption-driven emission of dislocation. The three mechanisms are different in principle, but they have one thing in common: no matter how the hydrogen gets into the material or what the circumstances are that the material degrades, the damage [15] is to some degree proportional to the amount of hydrogen in the material. Moreover, scientists are increasingly converging on the argument that there is a critical distance (X_{crit}) before the tip of the crack in the Fatigue Process Zone (FPZ) at which hydrogen damage (nucleates) or accumulates [16] [17] [18]. According to experiments done with FCG in many different conditions, assuming that the FCGR can be achieved through a multiplicative relation between the driving force of FCG and the inhibitory diffusion process (which could be a stress-assisted process), which can be determined as follows:

$$\frac{da}{dN} = A \cdot \Delta K^n \cdot F(env) \quad (1)$$

where, A and n represent specific constants of the material, ΔK denotes the range of the stress intensity factor, and $F(env)$ is a functional model that links the interaction between diffusion kinetics and detrimental environments, corresponding to FCG in hydrogen environments, for which relevant models have also been proposed [19] [20] [21].

Currently, two models for FCG in hydrogen environments have been proposed to study the simultaneous occurrence of multiple types of damage mechanisms. The first is the linear superposition model [22] [23], which assumes that each increment of crack growth occurs independently and is the sum of the contributions from non-interacting mechanisms. This model is used for solving the FCGR, and its expression is as:

$$\frac{da}{dN_{Total}} = \sum \frac{da}{dN_i} \quad (2)$$

In this context, the subscripts $Total$ and i represent the overall crack growth and any arbitrary number of independent mechanisms, respectively. The second approach is the cumulative damage model [24] [25], which assumes that multiple concurrent damage mechanisms "compete" with each other; thus, any single mechanism may dominate the overall deformation, or the total deformation may result from the interaction of multiple mechanisms. The general framework expression of this model is given by:

$$D_{Total} = \sum D_i \quad (3)$$

where D_{Total} represents the total damage caused by all the mutually "competing" mechanisms, while D_i denotes the damage caused by each individual damage mechanism. The linear superposition model treats the deformation mechanisms as occurring in parallel, whereas the cumulative damage model assumes that independent deformation mechanisms occur in series, in which case the cumulative effect may include the interactions between damage mechanisms. When applied to life prediction, the cumulative damage model becomes:

$$N_f = [D_{\text{Total}}]^{-1} = \left[(N_{f1})^{-1} + (N_{f2})^{-1} \right]^{-1} \quad (4)$$

where N_f represents the predicted number of failure cycles, while N_{f1} and N_{f2} denote the number of failure cycles for two independent damage mechanisms. The fundamental concept of this model is that failure (separation) of the material occurs when the total damage equals one [16]. For FCG consisting of two competing crack growth mechanisms $\frac{da}{dN_{f1}}$ and $\frac{da}{dN_{f2}}$, the cumulative damage model can be expressed as:

$$\frac{da}{dN_{\text{Total}}} = \left[\left(\frac{da}{dN_{f1}} \right)^{-1} + \left(\frac{da}{dN_{f2}} \right)^{-1} \right]^{-1} \quad (5)$$

In both of these approaches, competing damage mechanisms may cause the FCG behavior to deviate from Paris's law, while the first linear superposition model is based on Paris's law and integrates the increments of crack growth under various mechanisms [26]. In the FCG model for pipeline steel in hydrogen environments, a calculation method for the FCGR has also been derived based on the mechanism of a linear superposition model.

2.2. Analysis of HA-FCG in Hydrogen Environments

According to the results of completed FCG experiments on pipeline base materials in hydrogen environments, there exists a threshold for the increase in HA-FCG rates. When the range of the stress intensity factor ΔK exceeds this threshold, the HA-FCG rate is observed to be higher than the FCG rate in the air [27] [28] [29]. Amaro et al. [16] further categorized the relevant data into multiple linear response regions for FCG based on the FCG experimental results of X100 pipeline steel in hydrogen environments, as shown in fig. 1.

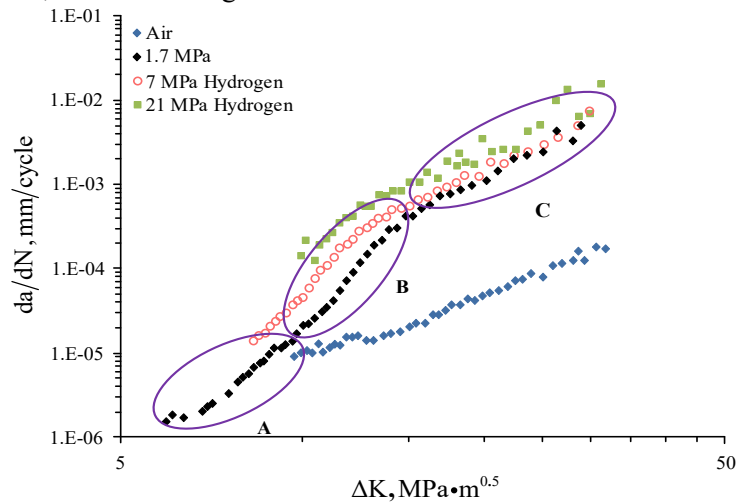


Fig. 1. Typical three-stage HA-FCG results for API X100 pipeline steel.

As shown in fig. 1, the crack growth of this material in a hydrogen environment can be divided into three regions. When $\Delta K < \sim 8 \text{ MPa m}^{1/2}$, a specific trend of HA-FCG is observed; when $\sim 8 \text{ MPa m}^{1/2} < \Delta K < \sim 15 \text{ MPa m}^{1/2}$, a different trend is noted, and when $\Delta K > \sim 15 \text{ MPa m}^{1/2}$, a third trend emerges. These three trends correspond to the regions referred to as "Air," "Transient," and "Steady-State," corresponding to regions A, B, and C, respectively. Analysis of the hydrogen-induced fatigue fracture surfaces in these three regions reveals that each state is produced by different dominant damage mechanisms, with each mechanism prevailing at different times. The response in region A is unaffected by hydrogen; thus, the fatigue surfaces generated in this region match those of tests conducted in air, primarily governed by pure fatigue mechanisms [30]. The FCG responses in regions B and C are influenced by hydrogen, and the transition between the FCG responses in these two regions is determined by the characteristic length scale x_{tr} . In HA-FCG, the characteristic length scale x_{tr} is a function of the FPZ, and the transitions between the linear trends of FCG are caused by the interaction between the crack growth length per cycle and the characteristic length scale of the material's microstructure. Additionally, the FPZ represents the region ahead of the crack tip, which experiences significant plastic deformation due to the combined effects of cyclic loading and high levels of hydrostatic pressure.

Furthermore, studies found that when the FCG is located within region B, $\frac{da}{dN}$ is

situated in the area of increased hydrogen concentration due to the $\frac{1}{r}$ dependence of

hydrostatic stress. Because these materials exhibit this specific FCG response under a limited amount of crack growth per cycle, this region is also referred to as the transient HA-FCG mechanism. Within this region, the hydrogen accumulation at the crack tip dominates the damage response of this HA-FCG mechanism, resulting in a more brittle response of the material compared to that in region A, which leads to FCG surfaces primarily characterized by crystalline facets.

Additionally, crack growth occurs in the FPZ and the associated region of increased hydrogen concentration within region A for each cycle. However, since the critical stress intensity factor K required for the onset of environment-assisted mechanisms has not yet been reached (the transition point away from air FCG) [31], HA-FCG does not exhibit an increase compared to air. When HA-FCG is in region C, its state

is referred to as the steady-state condition. When the crack growth per cycle $\frac{da}{dN}$

exceeds the transition length x_{tr} of the FPZ and is accompanied by enhanced hydrogen accumulation, crack growth is primarily influenced by the far-field hydrogen accumulation within the material. Moreover, the FCG surfaces under this mechanism are very similar to those tested in air. Therefore, the HA-FCG response is predominantly governed by traditional fatigue mechanisms.

The assumed interaction between crack growth and the FPZ is illustrated in fig. 2. Fig. 2(a) depicts the transient HA-FCG associated with region B, where it is evident that the FCG increases when the crack growth per cycle occurs within a dimension

of x_r of the FPZ. In this scenario, the hydrogen accumulated at the crack tip dominates the damage response under transient conditions. Fig. 2(b) illustrates the relationship between the cyclic crack growth and the FPZ associated with region C. Specifically, in this state, the crack extends through the FPZ and beyond it with each cycle. It can be observed that, in this case, intergranular crack growth is significantly more prevalent than transgranular crack growth, resulting in FCG surfaces generated under these conditions being more similar to the FCG surfaces of the material tested in air.

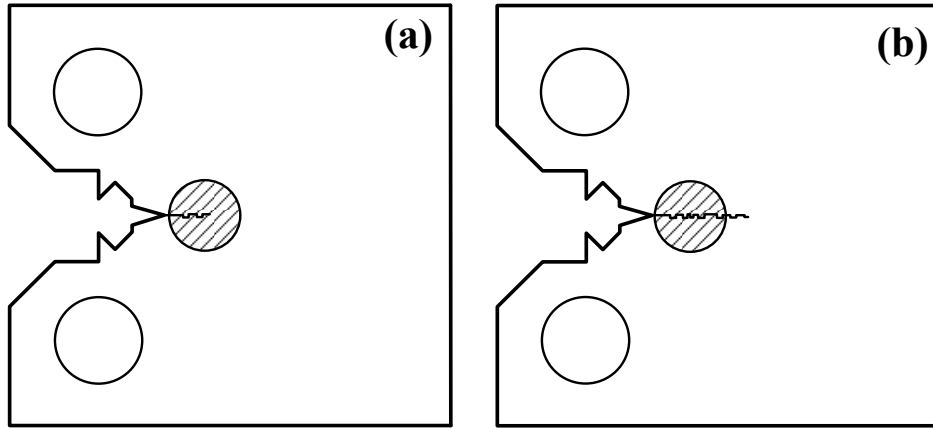


Fig. 2. Hydrogen-induced cracking: (a) Transient HA-FCG state (Region B) (b) Steady-state HA-FCG state (Region C).

2.3. Fatigue Crack Growth model in hydrogen environments

The general framework of FCG superposition has been successfully applied to various environments, including oxidative environments [32] [33], corrosive environments [34], viscoplastic deformation induced by high temperatures [35], thermal-mechanical fatigue [36], and crack growth data categorized by microstructural considerations [32]. For the study of FCG models in hydrogen environments, the FCG superposition strategy remains applicable. As described in Section 2.2, if regions B and C are classified as fatigue induced by the environment, it can be assumed that the incremental crack growth at the crack tip due to HA-FCG consists of contributions from both air fatigue and environmental fatigue (HA). Consequently, the FCGR relationship can be calculated as:

$$\frac{da}{dN_{\text{Total}}} = \frac{da}{dN_{\text{air}}} + \delta(P_H - P_{H_{th}}) \frac{da}{dN_H} \quad (6)$$

where the subscripts "air" and "H" represent the contributions to the total crack growth rate from fatigue in air and fatigue in a hydrogen environment, respectively. δ denotes the Heaviside step function, P_H represents the threshold hydrogen pressure, and when the environmental hydrogen pressure P_H exceeds the threshold $P_{H_{th}} = 0.02 \text{ MPa}$ [27], the Heaviside step function δ activates the hydrogen FCG response.

The Paris equation is a traditional FCG model based on the principles of fracture mechanics, primarily describing the relationship between the crack growth rate during the stable growth phase and the amplitude of the stress intensity factor. Equation (7) describes the scenario of FCG in air and represents the calculation method for the $\frac{da}{dN_{\text{air}}}$ term in equation (6). The basic form of the Paris equation is given by:

$$\frac{da}{dN_{\text{air}}} = A \Delta K^b \quad (7)$$

where, $\frac{da}{dN_{\text{air}}}$ represents the crack growth rate, ΔK denotes the range of the stress intensity factor. A and b are constants fitted based on experimental data.

What's more, the calculation method for $\frac{da}{dN_H}$ incorporates the separation assumption of deformation modes in bilinear HA-FCG results. This approach allows for a distinct analysis of the contributions of different deformation mechanisms under hydrogen-enriched conditions. It can be calculated as:

$$\frac{da}{dN_H} = F[a \Delta K^b [H]] = F[a \Delta K^b P_H^m \exp((-Q + \sigma_h v)/RT) t^a] \quad (8)$$

In which, a is a functional relationship, H is the equilibrium hydrogen concentration, P_H is the hydrogen pressure, Q is the activation energy, σ_h is the hydrostatic pressure, v is the universal gas constant; T is the absolute temperature. The functional form of the equation assumes. The explanation of (8) is that FCG is increased by increasing the concentration of hydrogen in the material. Although this concept can be easily accepted, according to the results of experiments, offered to the literature, the nature of the interaction can be multiplicative as shown in the formula below. (8) is entirely empirical (because even the particular relations between the hydrogen concentration, stress, and inelastic strain at the crack tip during HA-FCG are not well understood yet).

Simple linear damage superposition is not an accurate representation of the response of HA-FCG in hydrogen environments and is key to understanding this phenomenon. In particular, HA-FCG can be regarded as the consequence of interaction between two hydrogen-assisted processes: one in which hydrogen accumulation at the crack tip prevails and results in hydrogen-dominated FCG. By comparison, the mechanism of the other effect is hydrogen-assisted and is mainly controlled by conventional air-fatigue damage processes. Recent research suggests that the interaction of the hydrogen-based damage mechanism and the damage mechanism linked more properly to the deformation condition at the crack tip is thought to be the cause of the HA-FCG response [18].

Modeling the two interacting HA-FCG mechanisms as occurring in parallel allows the overall response $\frac{da}{dN_H}$ in a hydrogen environment to be influenced by both the dominant mechanism and the less dominant mechanism. The expression for this

relationship is shown below.

$$\frac{da}{dN_H} = \left[\left(\frac{da}{dN_{P_H}} \right)^{-1} + \left(\frac{da}{dN_{\Delta K}} \right)^{-1} \right]^{-1} \quad (9)$$

where, $\frac{da}{dN_{P_H}}$ represents the HA-FCG response dominated by hydrogen accumulation in the FPZ, while $\frac{da}{dN_{\Delta K}}$ denotes the HA-FCG response governed by the deformation at the crack tip. The HA-FCG response dominated by hydrogen accumulation in the FPZ can be calculated as:

$$\frac{da}{dN_{P_H}} = a_1 \Delta K^{B_1} \left(P_H^{m_1} \exp \left(\frac{-Q + V \sigma_h}{RT} \right) \right)^{d_1} \quad (10)$$

where, Q represents the activation energy for hydrogen diffusion ($Q = 27.1$ kJ/mol) [37]; V denotes the partial molar volume of hydrogen in the metal ($V = 2.0 \times 10^{-6}$ m³/mol) [38] [39]; R is the universal gas constant; T is the absolute temperature; σ_h refers to the hydrostatic stress at the critical distance ahead of the crack tip; P_H is the environmental hydrogen pressure; a_1 , B_1 , m_1 and d_1 are fitting parameters. Due to the lack of better alternative methods, the stress intensity factor is used here to capture information related to the stress and deformation state at the crack tip. Therefore, the HA-FCG response dominated by the deformation at the crack tip can be described by [31]:

$$\frac{da}{dN_{\Delta K}} = a_2 \Delta K^{B_2} \left(P_H^{m_2} \exp \left(\frac{-Q + V \sigma_h}{RT} \right) \right)^{d_2} \quad (11)$$

where a_2 , B_2 , m_2 and d_2 are fitting parameters, while all other parameters are defined as previously stated. However, studies have shown that regardless of the environmental hydrogen pressure, the HA-FCG results converge at larger values of ΔK , thereby minimizing the influence of the terms within the parentheses and causing the value of d_2 to approach 0 [23][40]. Consequently, the following functional form is proposed for the stress intensity factor-driven HA-FCG:

$$\frac{da}{dN_{\Delta K}} = a_2 \Delta K^{B_2} \quad (12)$$

Based on the steady-state HA-FCG response reflected in equation (10), researchers have found that a simplified engineering model can be developed to meet the specifications of practical engineering applications [16]. The simplified model divides the FCG response into three components, applying a power law relationship to each part, and coupling these three components within the same mathematical framework as the full model [32]. Specifically, the architecture of the simplified model is analogous to that of the full model, as shown in:

$$\frac{da}{dN_{\text{total}}} = \frac{da}{dN_{\text{air}}} + \delta (P_H - P_{H_{th}}) \frac{da}{dN_H} \quad (13)$$

where the first term $\frac{da}{dN_{\text{air}}}$ is the same as equation (6) calculated using equation (7), and the HA-FCG response $\frac{da}{dN_H}$ continues to be described by equation (9), but the expressions for its subcomponents are simplified as follows:

$$\begin{cases} \frac{da}{dN_{P_H}} = a_3 \Delta K^{B_3} \\ \frac{da}{dN_{\Delta K}} = a_4 \Delta K^{B_4} \end{cases} \quad (14)$$

where a_3 , a_4 , B_3 and B_4 are the values of the fitting parameters. By substituting equations (9), (11), and (14) into equation (13), the simplified calculation model for the FCGR in a hydrogen environment can be obtained, as shown in equation (15).

$$\frac{da}{dN_{\text{total}}} = A \Delta K^b + \delta (P_H - P_{H_{th}}) \left[(a_3 \Delta K^{B_3})^{-1} + (a_4 \Delta K^{B_4})^{-1} \right]^{-1} \quad (15)$$

where δ represents the Heaviside step function, with its expression given in equation (16). P_H denotes the hydrogen pressure, and $P_{H_{th}}$ is the threshold hydrogen pressure, which is set at 0.02 MPa in this case.

$$\delta = \begin{cases} 0 & P_H < P_{H_{th}} \\ 1 & P_H \geq P_{H_{th}} \end{cases} \quad (16)$$

3. Assessment of Hydrogen-Induced Fatigue Crack Growth rate based on PINN

As can be seen in the discussion in Section 2, the present determination of FCGR caused by hydrogen often involves the use of raw data obtained by the use of complex physical experiments. These tests require both human and financial resources, are time-consuming, and do not increase the efficiency of the FCGR assessment. Standard techniques used to estimate FCGR will mainly take the stress intensity factor at the crack tip and material parameters. Though greater considerations include the evaluation of hydrogen-induced FCGR, other environmental parameters, such as temperature, pressure, microstructure, and load frequency, are not taken into account. In addition, the coupling effects of the various physical fields remain a problem that has not been resolved.

As a solution to these challenges, surrogate models can be used to combine the multidimensional data and nonlinear behavior of the crack growth rate [41] [42]. PINN is a unified approach that uses data- and physics-driven methods to provide high accuracy, efficiency, and the capacity to model non-linear associations. Thus, PINN would be effective in helping to assess the effects of hydrogen on FCGR in order to address the following problems: 1) developing surrogate models at different scales; 2) offsetting the inability to find raw information in complex structures; 3) harmonising the prediction of growth rates of small cracks, physically small cracks, and long cracks; and 4) increasing the physical validity and interpretability of FCGR

measurement. The purpose of this approach will be to enhance the efficiency, fidelity, and applicability of crack growth rate analyses in hydrogen regimes, thus addressing the weaknesses of the classical theoretical analyses in terms of treatment of the multivariate interaction, scales-of-scales, and uncertainty assessment [43].

3.1. Factors influencing Fatigue Crack Growth

To include several items that influence hydrogen-assisted FCGR in the loss function of a PINN model, why not define a composite loss function that incorporates these items. This may include trading off each factor according to its contribution to the crack growth so that the model adequately reflects the compound interactions among them. Hydrogen transportation is commonly stored and transported as compressed gas [44]. The solubility of hydrogen in the metal lattice according to the law of Sievert is directly proportional to the partial pressure of the gas. The extent of fatigue degradation, is associated with the density of the atoms of hydrogen in the metal lattice and is thus too, dependent upon the hydrogen pressure [45]. The correlation between the FCGR and pressure in a definite pressure range may be characterized as [46].

$$\frac{\frac{da}{dN_H}}{\frac{da}{dN_{Total}}} = 1 + N \cdot P_{H_2}^{0.36} \quad (17)$$

Where N and P_{H_2} are coefficients which take into consideration the kind of steel and the partial pressure of gas respectively. The dependence of pressure on FCGR is dependent on the scope of the stress intensity. The pressure changes particularly at environments with high ΔK have a minor effect on FCG. On the other hand, at low ΔK an increase in H_2 correspondingly leads to an increase in FCGR.

Temperature has a major effect on the hydrogen concentration of materials, which is subject to hydrogen diffusivity, in addition to the overall hydrogen embrittlement process. The temperature rise tends to accelerate the rate of diffusion of hydrogen, and this causes a rise in the concentration of hydrogen and a rise in FCGR. The fact that the diffusion rate of hydrogen atoms is less in the low temperatures has been supported by many experiments [47] [48] [49] [50], which can be attributed to the following manner: The diffusion rate of hydrogen atoms is lower in the low temperatures which makes it difficult to have high movement of hydrogen. As a result, the scores of difficulties arise in case of hydrogen concentration at the critical points even when materials are subjected to deformation. Conversely, higher temperatures will aid in desorbing and releasing the hydrogen atoms and reduce the ability to store hydrogen in the sections of the material that were of importance.

Hydrogen purity has a significant effect on its adsorption and absorption processes which means it will have a considerable impact on the FCGR. It may be detrimental through certain impurities that may inhibit the absorption of hydrogen into bulk materials either by forming surface oxides or by adsorbing into their surface. At reduced loading frequencies, the hydrogen atoms are getting more time to diffuse on

fatigue cracks into the metallic matrices exaggerating the crack propagation. This subsequently makes the frequency dependence of FCGR a very important matter in the low-pressure condition but not in high-pressure conditions as has been illustrated in literature [51] [52] [53]. Better still, the fewer the frequency the more time the hydrogen atoms have to travel through fatigue cracks to the metal. Hence, frequency dependence of FCGR is to be taken into account with low pressures. It has however been revealed to decrease in high pressures [54] [55]. Besides the above the following factors can affect FCGR, pressure ratio, the composition of composite metal materials, the nature of the microstructure material as well as the accuracy of equipment manufacture. Therefore, the PINN model has to consider these factors when forming the model to improve the accuracy of FCGR judgement.

3.2. Physics-Informed Neural Networks based on Hydrogen-Induced Fatigue Models]

By simultaneously considering both physical loss and data loss, the total loss function for the overall PINN model is constructed as follows:

$$\min: \text{Loss}_T = (1-w)\text{Loss}_{NN} + w\text{Loss}_p \quad (18)$$

where Loss_T represents the loss function of the overall PINN, while w denotes the weight parameter used to maintain the balance between network predictions and physical constraints. Loss_{NN} indicates the data loss of the neural network, and Loss_p represents the physical loss considered during the PINN simulation fitting process. The mathematical loss is given by:

$$\text{Loss}_{NN} = \frac{1}{n} \sum_{i=1}^n (N_p - N_f)^2 \quad (19)$$

where N_p represents the fatigue life predicted by the neural network, while N_f denotes the fatigue life obtained from experiments. The data loss aims to minimize the prediction error of the constructed network model, thereby approximating the experimental fatigue life.

The physical loss is calculated based on the error between the predictions of the neural network and the FCG model equation (15) derived in Section 2.3:

$$\text{Loss}_p = \sqrt{\frac{\sum_{i=1}^m \left(\left(\frac{da}{dN} \right)_{NN} - \left(\frac{da}{dN} \right)_p \right)^2}{m}} \quad (20)$$

where Loss_p represents the physical loss function constructed from the hydrogen-induced FCG model, i denotes the i -th set of input data, and m indicates the size of the data set. The loss is calculated using the Root Mean Square Error (RMSE) to minimize the discrepancy between the fatigue life predictions provided by the neural network model [56] [57] and those predicted by the crack growth model [58].

By incorporating the factors influencing FCG described in Section 3.1 as input information for the PINN, a high-accuracy PINN is established to describe the nonlinear and complex mapping relationship between fatigue life N and the key

factors influencing crack growth:

$$N_f = nn(p_{H_2}, \rho, H, \Delta\sigma) \quad (21)$$

where $nn(\bullet)$ represents the nonlinear mapping function established by the neural network, P_{H_2} denotes the partial pressure of the gas, ρ indicates the stress ratio, H represents the frequency, and $\Delta\sigma$ denotes the externally applied load.

Furthermore, during the training process of the PINN model, the loss is iteratively updated, and the weights and biases within the network are adjusted based on the loss values. According to the definition of artificial neural networks, the input data is transmitted through multiple layers, ultimately reaching the output layer to produce the output results. Each node (neuron) in a layer receives inputs from the previous layer and processes these inputs through a linear combination followed by an activation function, as illustrated in equation (22).

$$y = NN(x) = f(w_3(f(w_2(f(w_1x + b_1)) + b_2)) + b_3) \quad (22)$$

where x represents the input vector, y denotes the output vector, and w_1 , b_1 , w_2 , b_2 , w_3 , b_3 represent weights and biases of the input layer to the hidden layer, hidden layers to hidden layers, and the hidden layer to the output layer, respectively. The activation function is represented by the function. The whole iterative approach is adopted by adopting the PyTorch platform, which makes it convenient to update weights and biases via the process of automatic differentiation and the Adam optimizer. In addition, the activation function is important in optimising the neural network. Some of the typical activation functions will be provided in Table 1; the ReLU function will be chosen as the activation function of the PINN model, owing to its efficient computation and nonlinear transformation capability. This allows the PINN model to better and faster merge physics laws and experimental evidence and get the required predictive outcomes.

Table 1. Common activation functions and their expressions

Activation functions	Expressions
Sigmoid function	$f(x) = \frac{1}{1 + e^{-x}}$
Hyperbolic Tangent (Tanh) Function	$f(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
Rectified Linear Unit (ReLU) Function	$f(x) = \max(0, x)$
Leaky ReLU Function	$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x & \text{if } x \leq 0 \end{cases}$
Parametric ReLU (PReLU) Function	$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha_i x & \text{if } x \leq 0 \end{cases}$
Exponential Linear Unit (ELU) Function	$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases}$
Softmax Function	$f(x_i) = \frac{e^{x_i}}{\sum_j e^{x_j}}$

In addition to the drops and falls of weights and biases in the artificial neural network model, the construction and learning rate are significant in the predictive outcomes of the model [59]. Particle Swarm Optimization (PSO) [60] [61] algorithm is applied in this study to optimise the number of the hidden neurons, the learning rate, as well as the weights used in equation (18) of the PINN model. The range of optimizations of every parameter is displayed in Table 2.

Table 2. Search optimization ranges for different parameters

Parameters	Search range
The number of neurons in the first hidden layer.	[10, 128]
The number of neurons in the second hidden layer.	[5, 64]
Learning rate	[0.001, 0.1]
w	[0.1, 1]

The entire process of the PINN model for training, optimization, and prediction is illustrated in fig. 3. After the training dataset is input into the model, the PSO algorithm is employed to adjust the network's structure and parameters. Once the model is trained, it proceeds to predict the results on the validation dataset.

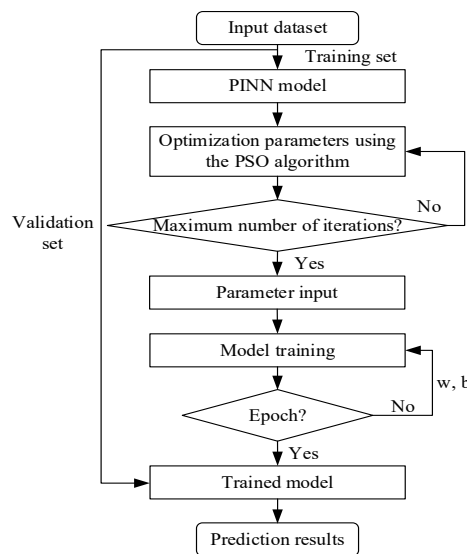


Fig. 3. Flowchart of the entire training and prediction process of the PINN model.

Therefore, the incorporation of physical information in the proposed PINN model primarily occurs in the loss function component. During the input stage, the training set is used concurrently to train both the physical and model and the ANN model. Subsequently, the loss function is constructed based on the output results from both models, allowing for continuous iteration to train the overall PINN model, as illustrated in fig. 4.

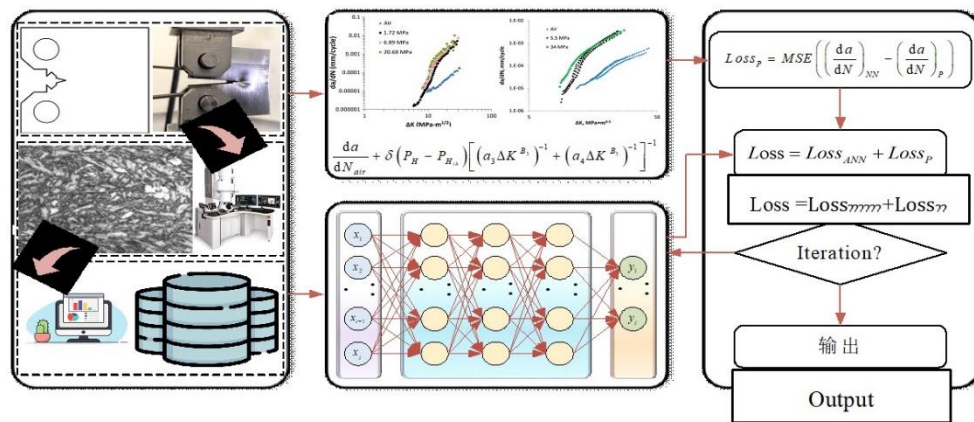


Fig. 4. PINN model structure diagram.

4. Validation of Fatigue Crack Growth Rate assessment example

4.1. Preprocessing of Experimental Data Set

To achieve accurate predictions of FCGR in a hydrogen environment, this study establishes and evaluates the HA-FCG model based on experimental data related to the FCG of pipeline steels in hydrogen environments, as reported in the existing literature. A total of 268 data points for API-X70 pipeline steel and 157 experimental data points for API-X100 pipeline steel were collected from previously published studies to form the dataset [62].

The two types of pipeline steels, API-X70 and API-X100, were subjected to FCG tests on compact tension specimens in the transverse-longitudinal direction, in accordance with the specifications of ASTM E647-08 [63]. The specimens used in the experiments were machined from commercially available pipes with a diameter of 1.3 meters and a thickness of 20.6 millimeters, which were manufactured using thermomechanical control processing and tested under as-received conditions. The dimensions of the specimens were 26.4 millimeters in length and 10.96 millimeters in width. The FCG experiments in air were conducted using a closed-loop 100 kN servo-hydraulic loading frame, while those in a hydrogen environment were performed in a 138 MPa pressure vessel. Force feedback was provided by a 44 kN load cell within the pressure vessel, and the hydrogen environment was generated through an electrolyzer using ultra-pure water. The frequency for the air environment was set at 10 Hz, whereas for the hydrogen environment, it was set at 1 Hz, with a stress ratio (R) of 1 for both environments. After the FCG experiments, the surface of the fatigue cracks was examined using a scanning electron microscope.

The FCG data for API-X100 and API-X70 pipeline steels under air conditions and various hydrogen pressure conditions are presented in Tables 3 and 4. Reference [16] determined the relevant parameters based on a simplified HA-FCG model, where the two parameters for API-X100 pipeline steel in air are $a = 9.83 \times 10^{-9}$ and $B = 2.8285$, while for API-X70 pipeline steel, the parameters are $a = 4.08 \times 10^{-9}$ and $B = 3.2106$,

with all other parameters set to zero. The parameters for the simplified model in a hydrogen environment are shown in Tables 5 and 6, which list the parameter values required for the HA-FCG model along with the experimental HA-FCG data. Additionally, the parameters related to FCG in air are the same as those in Tables 3 and 4.

Table 3. Partial HA-FCG Data for API-X100 Pipeline Steel in Air

Statistical parameters	Input parameters			Target variables
	ΔK (MPa•m ^{1/2})	Stress ratio R	Frequency H	$\frac{da}{dN}$ $\left(\frac{\text{mm}}{\text{cycle}}\right)$
Mean	18.0384	0.5	1	4.8120×10^{-5}
Minimum	9.5159	0.5	1	8.8313×10^{-6}
Maximum	31.7317	0.5	1	1.7570×10^{-4}

Table 4. Partial HA-FCG Data for API-X70 Pipeline Steel in Air

Statistical parameters	Input parameters			Target variables
	ΔK (MPa•m ^{1/2})	Stress ratio R	Frequency H	$\frac{da}{dN}$ $\left(\frac{\text{mm}}{\text{cycle}}\right)$
Mean	22.5003	0.5	1	1.2065×10^{-4}
Minimum	11.7301	0.5	1	9.7143×10^{-6}
Maximum	42.8129	0.5	1	5.8257×10^{-4}

Table 5. Partial HA-FCG Data for API-X100 Pipeline Steel under Different Conditions

Statistical parameter s	Input parameters						Target variables
	ΔK (MPa•m ^{1/2})	P_H (MPa)	a_3	B_3	a_4	B_4	$\frac{da}{dN}$ $\left(\frac{\text{mm}}{\text{cycle}}\right)$
Mean	14.6861	8.4860	1.1045×10^{-11}	8.1660	1.13×10^{-7}	3.2685	9.9764×10^{-4}
Minimum	5.9554	1.72	3.92×10^{-15}	6.4822	3.09×10^{-8}	3.05	1.4872×10^{-6}
Maximum	29.9588	20.68	4.09×10^{-11}	9.5469	2.4×10^{-7}	3.5035	1.0041×10^{-2}

Table 6. Partial HA-FCG Data for API-X70 Pipeline Steel under Different Conditions

Statistical parameter s	Input parameters						Target variables
	ΔK (MPa•m ^{1/2})	P_H (MPa)	a_3	B_3	a_4	B_4	$\frac{da}{dN}$ $\left(\frac{\text{mm}}{\text{cycle}}\right)$
Mean	14.7246	13.9626	2.2873×10^{-14}	9.5966	8.4845×10^{-7}	3.4445	6.6612×10^{-4}
Minimum	8.6932	5.51	1.31×10^{-15}	8.812	2.53×10^{-8}	2.9292	2.3574×10^{-6}
Maximum	27.5397	34.71	7.58×10^{-14}	9.9163	2.31×10^{-7}	3.6545	3.6399×10^{-3}

To tackle a wide range of contradictions that tend to occur in data of varied magnitude, such as missing values, noise, outlier and redundant features, one must standardise the raw data before processing. It will improve the interpretability and flexibility of the PINN model and increase the efficiency and quality of model development. Usually used ways to normalise data are:

Z-score normalisation is sometimes called zero-mean standardisation, and it mainly converts the data to a distribution in which the mean = 0, and the standard deviation = 1. This approach works well with most machine learning models and data analysis. The normalisation operation is provided by:

$$x' = \frac{x - \mu}{\sigma} \quad (23)$$

where x' represents the normalized input sample features, x denotes the unprocessed raw input sample features, μ is the mean of the data, and σ is the standard deviation of the data.

(2) Max normalization normalizes the range of the data to $[-1, 1]$ by dividing each feature in the original dataset by its absolute maximum value. The normalization function is given by:

$$x' = \frac{x}{|x_{\max}|} \quad (24)$$

where $x_{\max}$ represents the maximum value in the dataset, and the meanings of x' and x are the same as in equation (23).

(3) The Min-Max normalization method: The primary idea is to linearly transform the data to a specified range (typically $[0, 1]$). Let x represent a particular feature in the input dataset; the calculation formula for Min-Max normalization is given by:

$$x' = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (25)$$

and where $x_{\min}$ is the minimum of the original input sample features, $x_{\max}$ is the maximum of the original input sample features, and the meanings of x' and x are the same as mentioned in equation (23).

With the case of FCGR of pipeline steel in a hydrogen condition, the Min-Max normalisation technique was used to pre-data the original dataset to improve their training efficiency and accuracy of the PINN model and maintaining similarity in the feature of the dataset and their simplicity to use.

4.2. Model Evaluation and Validation

In order to analyse the proposed PINN model and ensure the comparison of the obtained predictions, one has to choose the applicable evaluation metrics. Since the size of FCGR under a hydrogen environment is comparatively small and has a slight oscillation, the conventional measures of mean-squared error are not of use. Thus, in this research, two measures of evaluation were used, RMSE and Mean Absolute Error (MAE) to measure the accuracy of the model. The two measures can be used

to determine that there are important errors in the model without increasing the scale of the errors, hence giving the true picture of the model's predictive performance. Their words are as follows:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^m \left(\left(\frac{da}{dN} \right)_{\text{actual}}^i - \left(\frac{da}{dN} \right)_{\text{pred}}^i \right)^2}{m}} \quad (26)$$

$$\text{MAE} = \frac{1}{m} \sum_{i=1}^m \left| \left(\frac{da}{dN} \right)_{\text{actual}}^i - \left(\frac{da}{dN} \right)_{\text{pred}}^i \right| \quad (27)$$

where $\left(\frac{da}{dN} \right)_{\text{actual}}^i$ and $\left(\frac{da}{dN} \right)_{\text{pred}}^i$ represent the actual and predicted values of the FCGR

in a hydrogen environment, respectively, and the superscript i denotes the i -th input vector, with m being the total number of input vectors.

As described in Section 3.2, considering the aim of obtaining more accurate predictions through the guidance of a physical model, the predictions made by the PINN model during its development process tend to align more closely with actual metrics and exhibit greater physical interpretability.

To illustrate the constraints imposed by the physical model on the PINN model throughout the iterative process, both datasets were divided into training and validation sets in an 80% to 20% ratio. Fig. 5 and 6 present the loss iteration results for the proposed PINN and related models on the training and validation sets of the API-X100 pipeline steel dataset, respectively. From the overall loss iteration trends of the models, it can be observed that after 7000 training epochs, the losses of both the artificial neural network and the PINN model gradually converge. The content of the two figures indicates that, with the introduction of physical constraints, the overall loss iteration process of the PINN model is smoother and exhibits more stable convergence, which can reduce the risk of overfitting.



Fig. 5. Variation of Losses under the X100 Training Set.

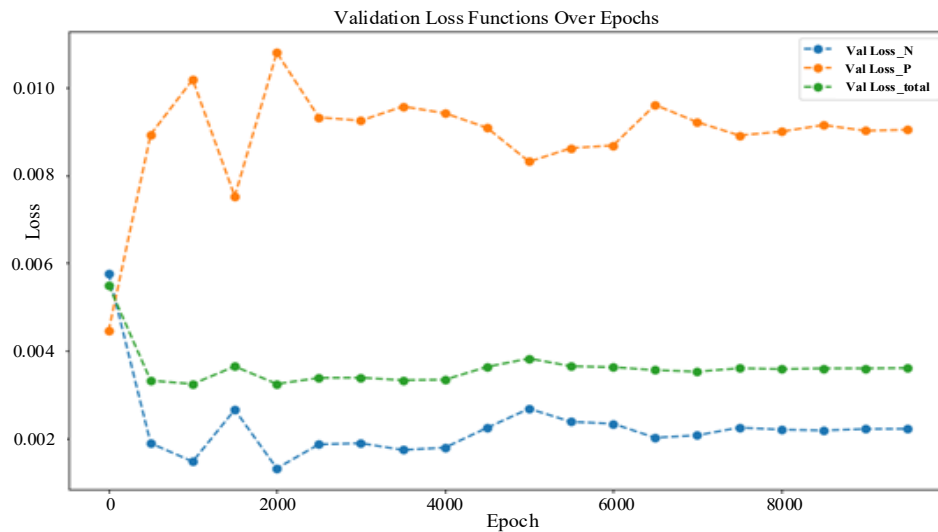


Fig. 6. Variation of Losses under the X100 Validation Set.

The results on the loss iteration of PINN and associated models on the training and validation sets comprising the API-X70 pipeline steel dataset are shown in fig. 7 and 8, respectively. The loss of the iteration is measured after every 500 epochs. Based on the entire iteration process, it can be noted that the loss of the different models on the training set approaches zero at around 500-training epochs. However, the models converge gradually after approximately 3500 epochs of training on the validation set, with the proposed model of PINN having a better stabilising iteration than the rest of the models.



Fig. 7. Variation of Losses under the X100 Validation Set.

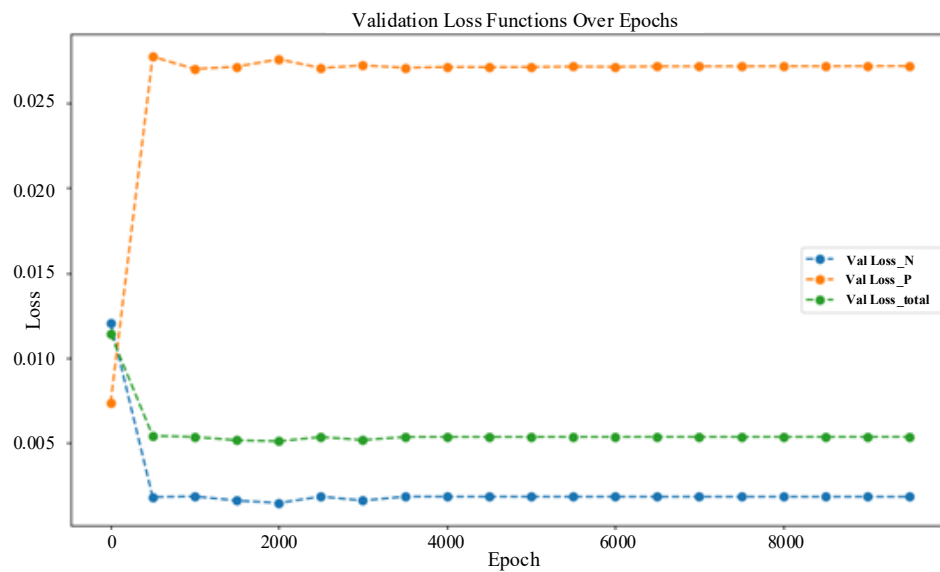


Fig. 8. Variation of Losses under the X70 Validation Set.

Furthermore, to validate the predictive performance of the proposed PINN model, a comparison was made between the prediction results of the original ANN model, the physical model, and the SVR model. Fig. 9 illustrates the comparison between the predicted values and the actual values for various models on the API-X100 pipeline steel dataset. The given fig. 9(a) shows that the Pinn model demonstrates a stronger ability to fit the original data compared to the other models, exhibiting superior predictive performance.

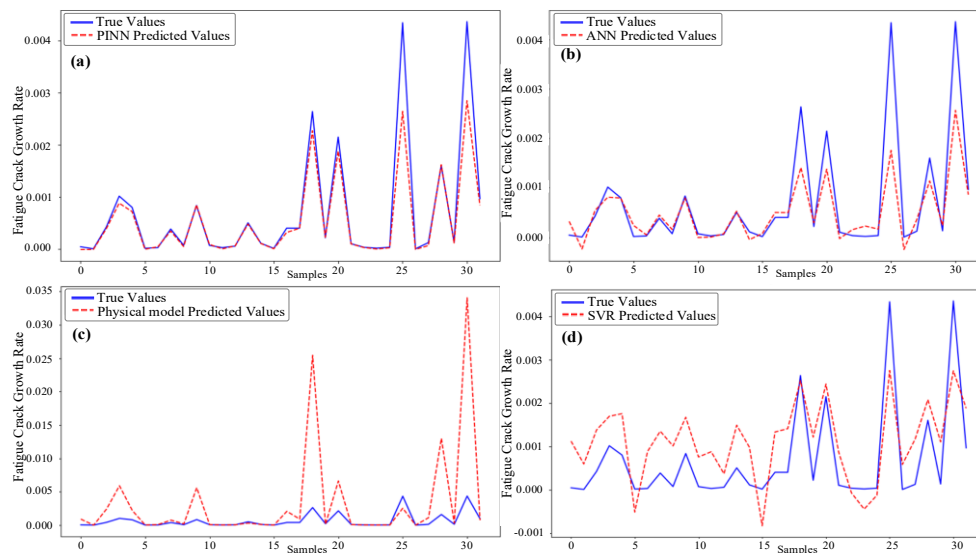


Fig. 9. Prediction Results of Various Models on the API-X100 Pipeline Steel Dataset: (a) PINN; (b) ANN; (c) Physical Model; (d) SVR.

In terms of error evaluation metrics, the proposed PINN model also demonstrates superior performance, exhibiting the smallest error values among the various comparison models, as shown in Table 7. Notably, the RMSE value of the SVR model is more than twice that of the PINN model, while the MAE value is over four times greater than that of the PINN model. The error metrics of the physical model are an order of magnitude higher compared to the other models, as can also be observed from the results in fig. 9. Although the error of the ANN model is relatively small, it still shows some disparity when compared to the PINN model.

Table 7. Performance Metrics of Different Models on the API-X100 Pipeline Steel Dataset

Heading level	RMSE	MAE
ANN	0.000423	0.000330
Physical Model	0.015178	0.005894
SVR	0.000855	0.000780
PINN	0.000326	0.000156

Fig. 10 presents the results of various models on the API-X70 pipeline steel dataset. On this dataset, the proposed PINN model aligns more closely with the validation set results compared to the other models, as shown in fig. 10(a).

Additionally, Table 8 displays the prediction metric values for different models on the API-X70 pipeline steel dataset. It can be observed from the table that the proposed PINN model achieves the smallest values for both metrics (RMSE and MAE), demonstrating a significant improvement in error compared to several other models. For instance, the error of the SVR model is three times that of the PINN model, while the prediction error of the physical model is on a different order of magnitude compared to that of the proposed model.

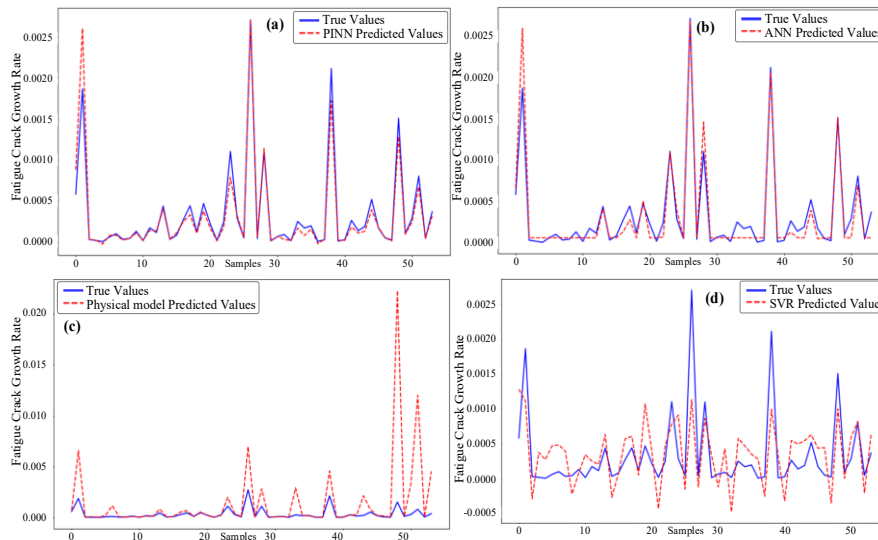


Fig. 10. Prediction Results of Various Models on the API-X70 Pipeline Steel Dataset: (a) PINN; (b) ANN; (c) Physical Model; (d) SVR.

Table 8. Performance Metrics of Different Models on the API-X70 Pipeline Steel Dataset

Heading level	RMSE	MAE
ANN	0.000179	0.000169
Physical Model	0.007307	0.002513
SVR	0.000420	0.000333
PINN	0.000122	0.000068

The FCGR of pipeline steel in a hydrogen environment primarily varies with changes in the range of the stress intensity factor ΔK . To analyze the predictive performance of the proposed PINN model under this relationship, the prediction results of all models are compared with the actual experimental results. For the API-X100 pipeline steel, the HA-HCG results at 34.71 MPa are selected for comparison, as shown in fig. 11. Compared to the other models, the prediction results of the PINN model are closer to the actual values, and it also demonstrates better fitting performance at lower FCGR values.

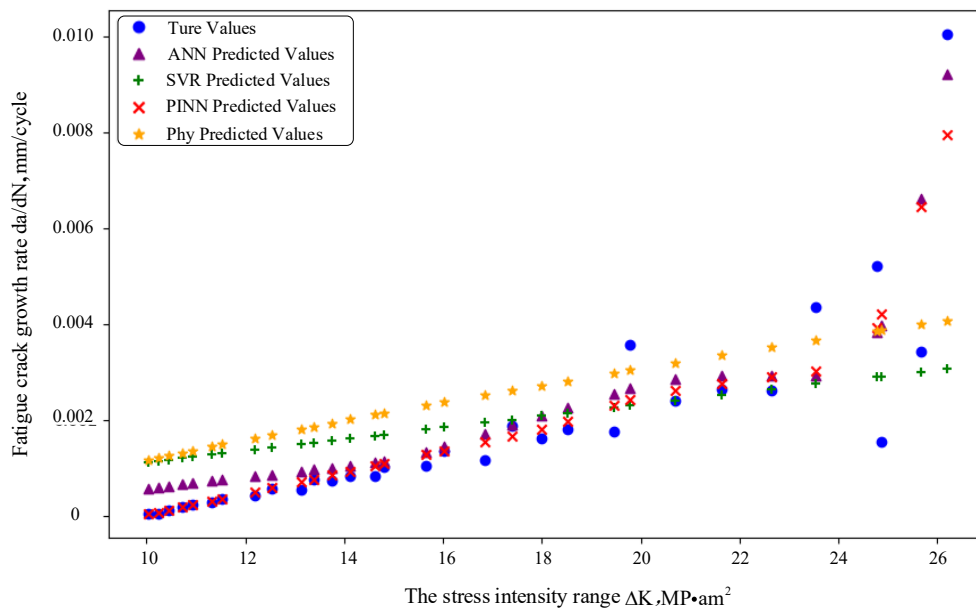


Fig. 11. HA-HCG Data and Model Prediction Results for X100 Pipeline Steel at a Hydrogen Pressure of 20.68 MPa.

For the API-X70 pipeline steel, the HA-HCG experimental results at a hydrogen pressure of 20.68 MPa are selected for comparison, as shown in fig. 12. From the prediction results of the various models, it can be observed that the PINN model more effectively captures the relationship between the HA-HCG rate and the range of the stress intensity factor ΔK .

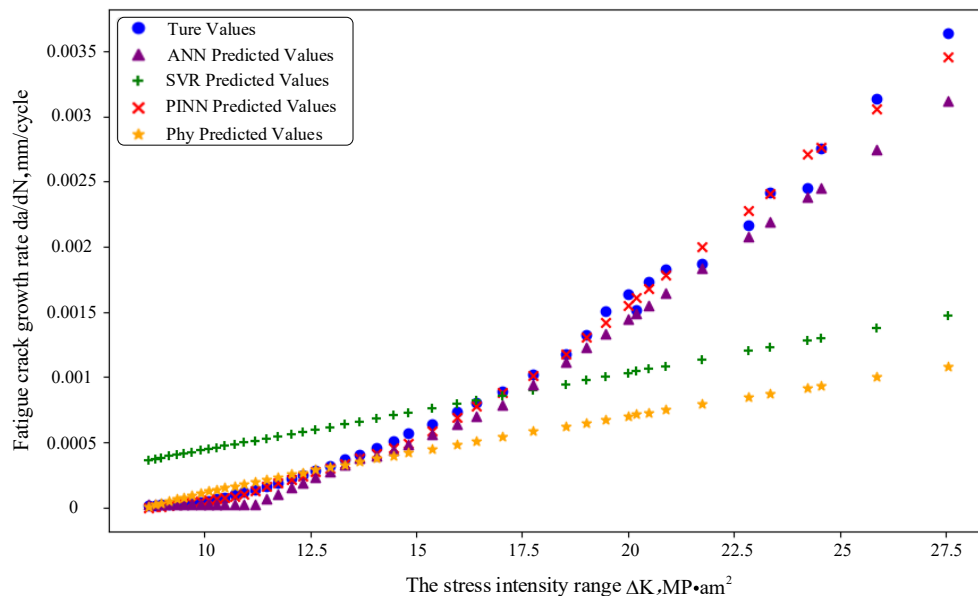


Fig. 12. HA-HCG Data and Model Prediction Results for X70 Pipeline Steel at a Hydrogen Pressure of 34.71 MPa.

5. Conclusion

This chapter introduces a characterization model for fatigue crack propagation in hydrogen environments, describing the calculation method for fatigue crack propagation rates in hydrogen environments. Based on the physical information representation of this model, it is embedded into the loss function of a neural network model, proposing a physical information-guided neural network to evaluate the fatigue crack propagation rate of pipeline steel materials in hydrogen environments. Furthermore, in the final evaluation results, the advantages of SVR and ANN models are integrated through Stacking ensemble learning, making the final evaluation results more accurate and interpretable. Fatigue crack propagation rate data of two types of pipeline steel, API-X70 and API-X100, in hydrogen environments were selected. The proposed model was compared and validated with PINN, ANN, SVR, and physical models. From the performance indicators and evaluation results of the selected models, the evaluation accuracy of the proposed model is superior to that of the other four models. Moreover, from the overall training and prediction process, the obtained evaluation results are more consistent with physical laws than those of purely data-driven machine learning models. Furthermore, the paper compares the iterative process of the proposed model with that of physical models and artificial neural network models. The results show that the proposed mode enters the convergence process faster, demonstrating the high efficiency of the proposed model in the evaluation of hydrogen-induced fatigue crack propagation rate.

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