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ACTIVE LEARNING ENHANCED STOCHASTIC SIZE-DEPENDENT DYNAMIC ANALYSIS OF THE PEROVSKITE SOLAR CELL

Luo Bo, and Jize Zhang*

Department of Civil and Environmental Engineering, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
First author e-mail: boluo@ust.hk

*Corresponding author e-mail: cejize@ust.hk

Abstract

The perovskite solar cell (PSC), recognized as a revolutionary advancement in next-generation photovoltaic devices, has emerged as one of the fastest-growing market competitors, characterized by its inherent micro-scale composite thickness. Investigating multi-scale vibrations of the PSC is a critical task for the overall dynamic system, as unfavourable responses can be minimized to the greatest extent possible. Furthermore, various physically inspired uncertainties inherently exist in practical engineering implementations. As a result, free vibration analysis that employs a deterministic model while neglecting intrinsic randomness is merely an approximation of realistic structural behaviour. Therefore, this research represents the first attempt to perform a stochastic size-dependent dynamic analysis of the PSC, taking into account multi-dimensional uncertainties with diverse distributions. An active learning technique, specifically the sequential design of experiment enhanced adaptive Kriging (SDOE-AKriging), is implemented to capture the underpinned and complex relationship between intrinsic uncertainties and the concerned size-dependent free vibration behaviour. Comprehensive statistical information regarding composite dynamic responses, encompassing the mean, standard deviation, coefficient of variation, probability density function, and cumulative distribution function, is furnished for structural safety assessment and reliability-based design. Numerical experiments demonstrate the superiority of the SDOE-AKriging over existing meta-model workhorses. Besides, the SDOE-AKriging is capable of delivering accurate vibration response forecasts for the PSC under rapidly changing conditions with tremendously alleviated computational toll, inspiring rapid information updates and timely dynamic behaviour monitoring in real engineering scenarios.

Keywords: Perovskite Solar Cell, Stochastic Size-dependent Vibration Analysis, Multi-scale Dynamics, Uncertainty Quantification, Active Learning.

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1 INTRODUCTION

The perovskite solar cell (PSC) with micro-scale thickness has instigated a remarkable technological advancement in third-generation photovoltaics, thanks to its favourable traits in easy production, high solar absorption efficiency, and plentiful raw materials [1–3]. Investigating the free vibration behaviour of the PSC is a key factor in analyzing the structural mechanical performance in practical applications [4–6]. Whereas, due to its ultra-thin characteristics, the structural properties and dynamic behaviour can become size-dependent [7]. In this context, traditional continuum theory in macro-mechanical analysis, which does not account for scale effects and internal material length scale parameters, may not provide accurate investigation results for composite responses [8]. In addition, numerous physically inspired uncertainties intrinsically exist in dynamic systems, and their effects on structural responses must be scrupulously quantified in composite safety assessment against reliability criteria [9]. Therefore, this work represents the first attempt to perform a stochastic size-dependent dynamic analysis of the micro-scale PSC under multi-dimensional uncertainties with various distributions. The refined shear deformation theory and modified strain gradient theory (MSGT) [10] are employed to investigate the size-dependent response incorporating scale effects. An active learning technique, specifically the sequential design of experiment enhanced adaptive Kriging (SDOE-AKriging) [11], is implemented to depict the underpinned and intricate relationship between input uncertainties and the focused size-dependent dynamic behaviour of the micro-PSC. Comprehensive statistical information regarding composite dynamic responses-including the mean, standard deviation (Std), probability density function (PDF), and cumulative distribution function (CDF)-is provided for structural safety assessment and reliability-based design. Numerical studies demonstrate the advantages of SDOE-AKriging against established meta-modelling tactics. Furthermore, the SDOE-AKriging is capable of offering accurate dynamic response forecasts for the PSC under swiftly varying environments while significantly reducing computational costs, inspiring rapid information updates and timely dynamic behaviour monitoring in real engineering scenarios.

2 SIZE-DEPENDENT FREE VIBRATION ANALYSIS OF THE PEROVSKITE SOLAR CELL

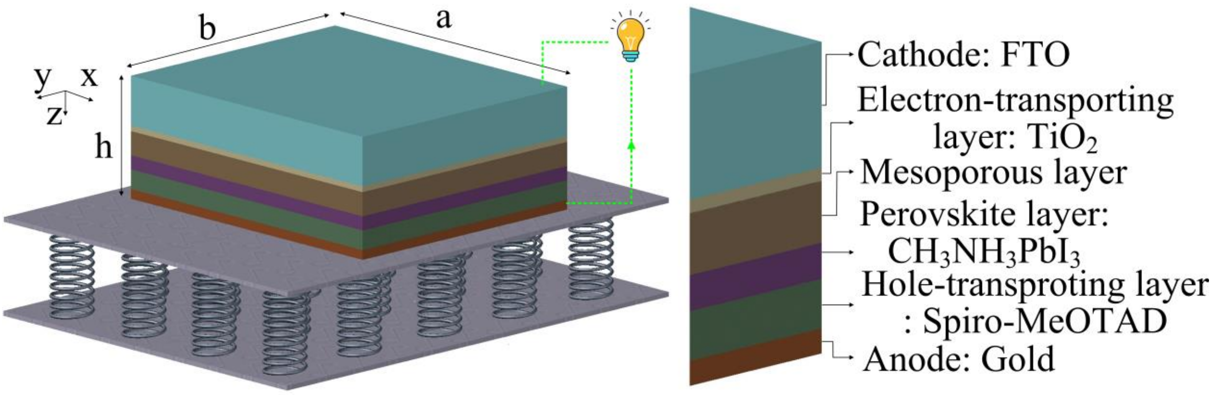

Figure 1: The micro-scale PSC on the Winkler-Pasternak elastic foundation and its architecture.

The architecture of the ultra-thin PSC is exhibited in Figure 1. The refined shear deformation theory [8] is leveraged and expressed as

$$\begin{cases} u_x(x,y,z,t) = u(x,y,t) - z\dfrac{\partial w_b}{\partial x} + (\dfrac{1}{4}z - \dfrac{5z^3}{3h^2})\dfrac{\partial w_s}{\partial x}, \\ u_y(x,y,z,t) = v(x,y,t) - z\dfrac{\partial w_b}{\partial y} + (\dfrac{1}{4}z - \dfrac{5z^3}{3h^2})\dfrac{\partial w_s}{\partial y}, \\ u_z(x,y,z,t) = w_b(x,y,t) + w_s(x,y,t). \end{cases} \tag{1}$$

Considering the inherent micro-scale thickness, the MSGT is implemented to describe the size-dependent effects. The constitutive expressions, which involve the classical stress tensor and higher-order stresses in the MSGT, are formulated as

$$\sigma_{ij} = \lambda\varepsilon_{mm}\delta_{ij} + 2\mu\varepsilon_{ij}, \tag{2}$$

$$p_i = 2\mu l_0^2\gamma_i, \tag{3}$$

$$\tau_{ijk}^{(1)} = 2\mu l_1^2\eta_{ijk}^{(1)}, \tag{4}$$

$$m_{ij}^{(s)} = 2\mu l_2^2\chi_{ij}^{(s)}, \tag{5}$$

where $\eta_{ijk}^{(1)}$, γ_i, and $\chi_{ij}^{(s)}$ indicate the deviatoric stretch gradient tensor, dilatation gradient tensor, and symmetric rotation gradient tensor, respectively. l_1, l_0, and l_2 denote the material length scale parameters associated with the deviatoric gradient, dilatation gradient, and symmetric rotation gradient, respectively.

Implementing the Navier scheme, Hamilton's principle, and Galerkin approach [12,13], the following formulation is obtained

$$([\overline{Kl}] - \omega_{mn}^2[\overline{Ml}])\{\Delta\} = \{0\}, \tag{6}$$

where

$$[\overline{Kl}] = \begin{bmatrix} Kl_{mn}^{11} & Kl_{mn}^{12} & Kl_{mn}^{13} & Kl_{mn}^{14} \\ Kl_{mn}^{21} & Kl_{mn}^{22} & Kl_{mn}^{23} & Kl_{mn}^{24} \\ Kl_{mn}^{31} & Kl_{mn}^{32} & Kl_{mn}^{33} & Kl_{mn}^{34} \\ Kl_{mn}^{41} & Kl_{mn}^{42} & Kl_{mn}^{43} & Kl_{mn}^{44} \end{bmatrix}, [\overline{Ml}] = \begin{bmatrix} Ml_{mn}^{11} & Ml_{mn}^{12} & Ml_{mn}^{13} & Ml_{mn}^{14} \\ Ml_{mn}^{21} & Ml_{mn}^{22} & Ml_{mn}^{23} & Ml_{mn}^{24} \\ Ml_{mn}^{31} & Ml_{mn}^{32} & Ml_{mn}^{33} & Ml_{mn}^{34} \\ Ml_{mn}^{41} & Ml_{mn}^{42} & Ml_{mn}^{43} & Ml_{mn}^{44} \end{bmatrix}. \tag{7}$$

The deterministic natural frequencies of the micro-PSC can be computed by resolving this eigenvalue task.

3 STOCHASTIC SIZE-DEPENDENT DYNAMIC ANALYSIS AND ACTIVE LEARNING TECHNIQUE

Taking into account the inherent physically inspired multi-dimensional uncertainties $\boldsymbol{\theta}_r$, the probabilistic eigenvalue equation in free vibration analysis represents

$$\{[\overline{Kl}(\boldsymbol{\theta}_r)] - \omega_{mn}^2[\overline{Ml}(\boldsymbol{\theta}_r)]\}\{\Delta\} = \{0\}. \tag{8}$$

For the above expression, classical analytical or mathematical schemes are nearly infeasible for this size-dependent stochastic dynamic problem. Hence, an effective active learning strategy, namely, the sequential design of experiment enhanced adaptive Kriging [11], is introduced to seize the sophisticated relationship between manifold multi-dimensional uncertainties and the concerned size-dependent free vibration behaviour of the PSC with scale effects, while furnishing sufficient statistical information on the composite response. The main components of the SDOE-AKriging encompass the Kriging meta-model, robust integrated mean squared error target function geared toward sequential experimental design, and advisable self-adjusting covariance matrix adaptation evolution strategy for addressing complex challenges in selecting optimal experiments and tuning hyperparameters.

4 NUMERICAL STUDIES

4.1 Verification

The free vibration behaviour of the PSC is examined and validated against published literature and commercial software (Table 1). As shown in the Table, the results of the presented work align well with established studies, confirming the accuracy of the developed dynamic analysis.

Mode(m,n)	Presented	[4]	ABAQUS	Max |relative difference|
(1,1)	525.7068	525.7047	525.7524 (1st)	0.008673%
(1,2)	1314.2659	1314.2697	1314.7312 (2nd)	0.03539%
(1,3)	2628.5280	2628.6030	2630.9904 (5th)	0.09359%
(2,3)	3417.0834	3417.0566	3419.4440 (7th)	0.06903%
(1,4)	4468.4885	4468.4342	4476.5511 (9th)	0.1801%

Table 1: Comparisons of natural frequencies of the PSC (Hz).

4.2 Numerical experiments

The physically inspired manifold uncertainties are incorporated and tabulated in Table 2. The crude Monte Carlo simulation (MCS) is performed with 10000 cycles to generate reference results for the stochastic size-dependent free vibration analysis of the PSC with scale effects. Figure 2 illustrates the accuracy improvement rates of different surrogate models as the training sample sizes increase. By virtue of the integrated active learning technique, the presented SDOE-AKriging demonstrates a superior accuracy enhancement speed compared to classical machine learning algorithms.

Random variables	E_{Au} (GPa)	$E_{\text{Spiro-MeOTAD}}$ (GPa)	$\nu_{\text{Perovskite}}$	$E_{\text{Perovskite}}$ (GPa)	$E_{\text{Mesoporous}}$ (GPa)	ρ_{TiO_2} (kg/m^3)	ρ_{TiO_2} (kg/m^3)	k_w (N/m^3)
Distribution	Lognormal	Lognormal	Beta	Normal	Lognormal	Normal	Normal	Normal
Mean	78	15	0.33	17.8	210.44	4230	6850	2000
Std	7.8	1.5	0.013	1.068	21.044	846	411	200

Table 2: Statistical information of inspected random variables in the micro-PSC.

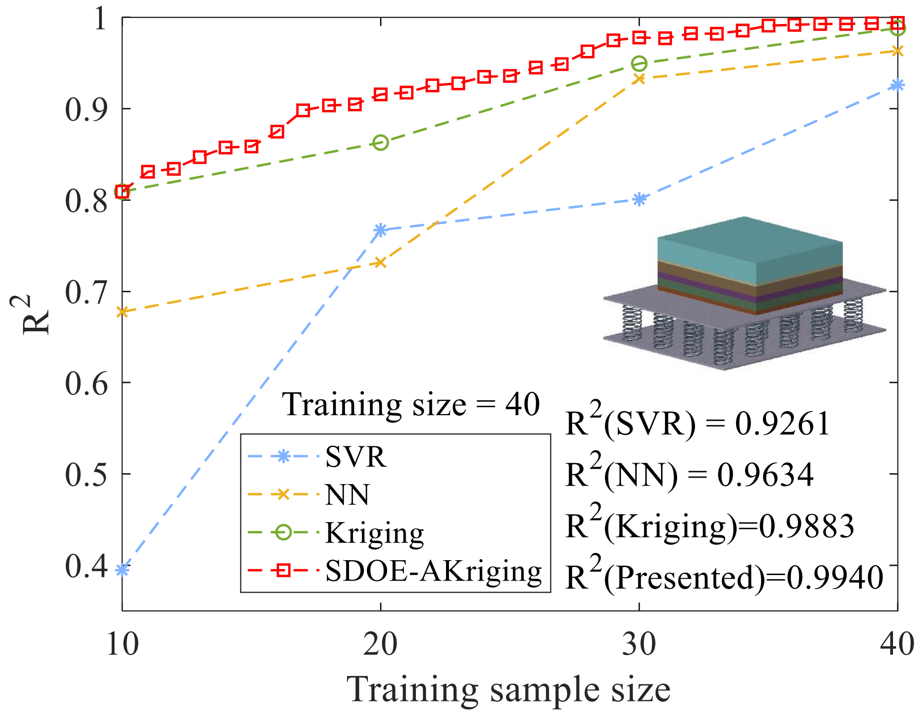

Figure 2: The R^2 of predicted size-dependent fundamental natural frequencies of the micro-PSC under different training sample sizes.

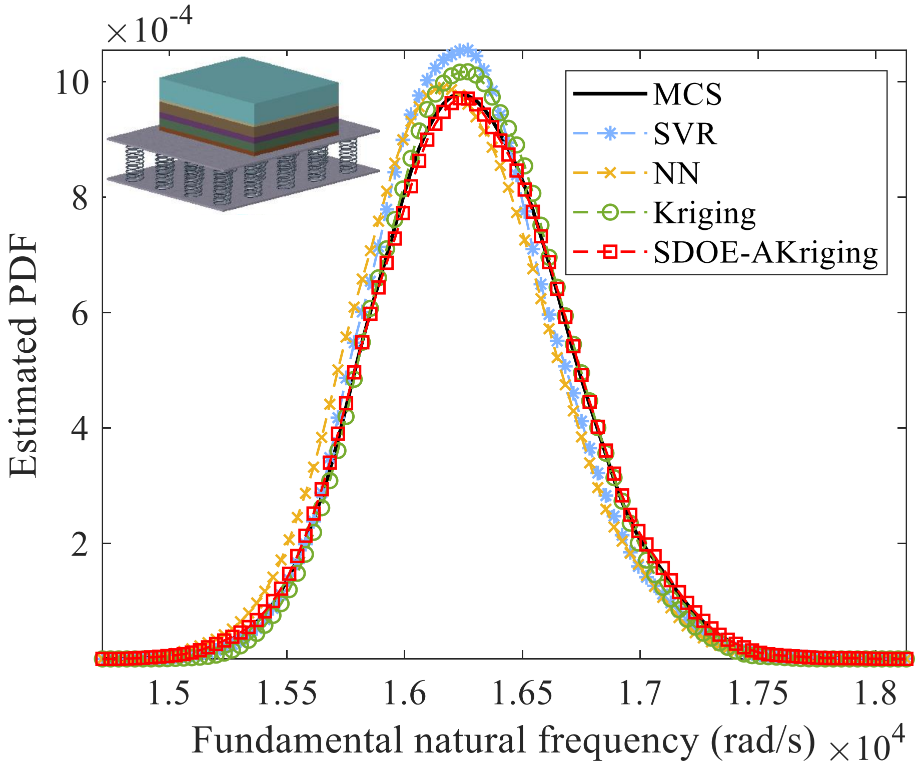

Figure 3: The estimated PDF of size-dependent fundamental natural frequencies of the micro-PSC.

The quantified statistical information of the PDF, CDF, and statistical moments of the mean and Std are manifested in Figures 3 and 4, as well as Table 3. By sequentially selecting a total of 40 optimal experiments, the presented SDOE-AKriging is competent to deliver accurately quantified statistical diagrams and moments of micro-composite dynamic behaviour, which match well with the brute-force MCS references. The higher R^2 value, superior Kolmogorov-Smirnov (K-S) statistic, and smaller relative errors in the mean and Std confirm the significant advantages of the SDOE-AKriging over existing meta-models. Furthermore, the computation costs of the MCS and presented active learning technique are 98.61min and 4.176min, respectively, implying the compelling efficiency of the proposed method.

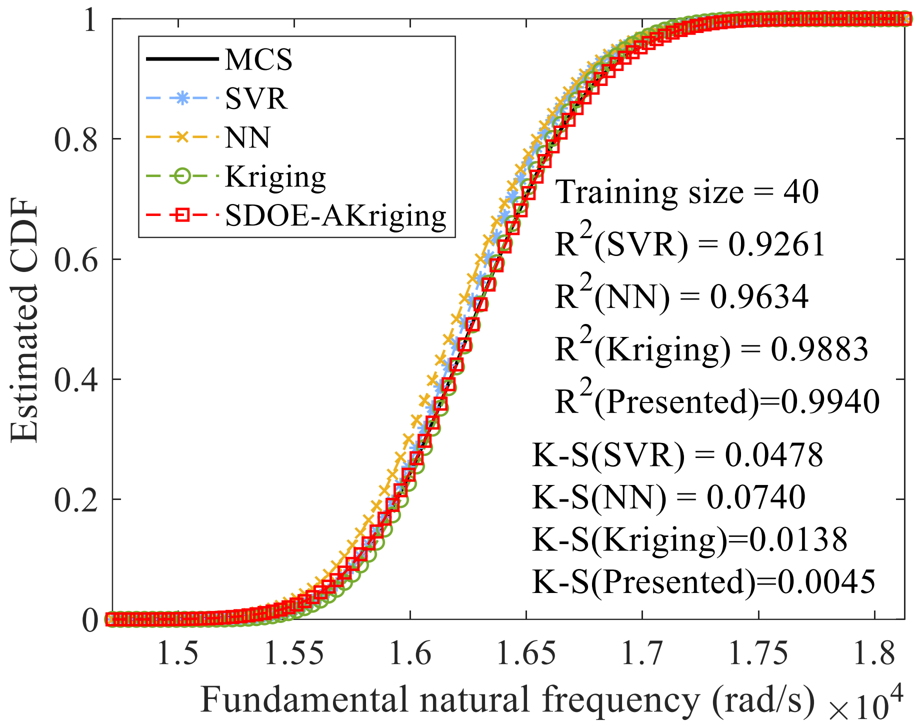

Figure 4: The estimated CDF of size-dependent fundamental natural frequencies of the micro-PSC.

Moment	Method	Fundamental natural frequency (rad/s)	Relative error against MCS(%)
Mean	SVR	1.6252×10^4	-0.2088%
	NN	1.6210×10^4	-0.4667%
	Kriging	1.6288×10^4	0.01228%
	SDOE-AKriging	1.6287×10^4	0.006140%
	MCS	1.6286×10^4	--
Std	SVR	3.7702×10^2	-5.5940%
	NN	3.9519×10^2	-1.0442%
	Kriging	3.7366×10^2	-6.4353%
	SDOE-AKriging	4.0236×10^2	0.7512%
	MCS	3.9936×10^2	--

Table 3: The estimated moments of size-dependent fundamental natural frequencies of the micro-PSC.

Moreover, the previously established SDOE-AKriging inherently possesses the merit of rapid information updates. Two arbitrary new sets of micro-PSC properties (shown in Table 4) are examined outside the original variation range. The results in Table 5 demonstrate the effectiveness and precision of the presented active learning technique in swift information updates under rapidly changing conditions, facilitating immediate composite decision-making in in real engineering scenarios.

Property	E_{Au} (GPa)	$E_{Spiro\text{-}MeOTAD}$(GPa)	$v_{Perovskite}$	$E_{Perovskite}$ (GPa)	$E_{Mesoporous}$ (GPa)	ρ_{TiO_2} (kg/m^3)	ρ_{TiO_2} (kg/m^3)	k_w (N/m^3)
Set1	90.43	13.29	0.3611	15.06	264.7	2494	5885	2571
Set2	60.56	18.93	0.2942	25.36	156.1	6460	8362	2068

Table 4: New input data sets of the micro-PSC properties.

Model comparison	SDOE-AKriging (×10^4 rad/s)	Physical free vibration analysis (PFVA, ×10^4 rad/s)	Relative error	SDOE-AKriging time (s)	PFVA time (s)
Set1	1.7777	1.7780	-0.01687%	0.000613	0.4317
Set2	1.4636	1.4659	-0.1569%	0.000276	0.3273

Table 5: Predicted size-dependent fundamental natural frequencies for new property input sets.

5 CONCLUSIONS

This research implements the stochastic size-dependent free vibration analysis of the micro-scale PSC under multi-dimensional uncertainties. With the aim of examining the scale effects on composite response, the refined shear deformation theory and modified strain gradient theory are utilized. An active learning strategy, specifically the sequential design of experiment enhanced adaptive Kriging, is incorporated to describe the underpinned and sophisticated relationship between various uncertainties and the focused size-dependent dynamic behaviour with tremendously reduced computational costs. Sufficient statistical information is provided, which is essential for the safety assessment and reliability-based design of micro-composites. Additionally, the superiority of the SDOE-AKriging over popular metamodels is confirmed through numerical experiments. Moreover, the developed tactic is capable of predicting the future size-dependent response of the PSC under rapidly varying environments, facilitating swift information updates in realistic engineering applications.

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