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Estimation of surface energies of hexagonal close packed metals using computational intelligence technique

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ABSTRACT

Surface phenomena such as corrosion, crystal growth, catalysis, adsorption and oxidation cannot be adequately comprehended without the full knowledge of surface energy of the concerned material. Despite these significances of surface energy, they are difficult to obtain experimentally and the few available ones are subjected to certain degree of inaccuracies due to extrapolation of surface tension to 0 K. In order to cater for these difficulties, we have developed a model using computational intelligence technique on the platform of support vector regression (SVR) to establish a database of surface energies of hexagonal close packed metals (HCP). The SVR based-model was developed through training and testing SVR using fourteen experimental data of periodic metals. The developed model shows accuracy of 99.08% and 100% during training and testing phase, respectively, using test-set cross validation technique. The developed model was further used to obtain surface energies of HCP metals. The surface energies obtained from SVR-based model are closer to the experimental values than the results of the well-known existing theoretical models. The outstanding performance of this developed model in estimating surface energies of HCP metals with high degree of accuracy, in the presence of few experimental data, is a great achievement in the field of surface science because of its potential to circumvent experimental difficulties in determining surface energies of materials.

1. Introduction

Creation of a unit surface area of a material requires an energy termed surface energy through which the stability of the surface is established. Surface phenomena such as corrosion, crystal growth, catalysis, adsorption and oxidation cannot be fully comprehended without the knowledge of surface energy of the concerned surface [1]. Limitation and difficulty of experimental techniques in determining surface energies of materials lead to daily development and extension of theoretical methods through which they can be easily estimated [2–9]. During the experimental determination of surface energy of materials, the material is heated to its melting phase so as to obtain surface tension of the concerned material. The extrapolation of the value of surface tension obtained to 0 K gives the surface energy of the specific material. Meanwhile, heating of materials to their melting phase is very difficult especially those that have high melting points, to crown it all, extrapolation of surface tension to 0 K subjects the experimental results to certain degree of inaccuracy [6]. Though, existing theoretical models such as embedded atomic method (EAM), equivalent crystal theory (ECT) and analytical equivalent crystal theory (AECT) and many others address this problem, many of them still have discrepancies in their estimates when compared to experimental values [3,4]. However, the use of the developed SVR-based model eliminates the issue of heating and extrapolation and gives excellent surface energy estimates close to experimental values. This is due to the ability of SVR to utilize the acquisition of complex relationship between the descriptors and surface energy in its generalization and prediction. Furthermore, the developed SVR-based model performs excellently well in the presence of few number of experimental data. First principle calculation of surface energy is computationally intensive and demanding and is usually employed for few elements [6]. Some semi-empirical methods are impressive but estimate surface energy lower than what is obtainable from the experimental data and first principle calculation [10–12]. Surface energies obtained from the developed SVR-based model are in excellent agreement with the generally accepted experimental values. The ability of this approach to give accurate estimation

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of surface energies in the presence of few experimental data, indicates its potential to circumvent the experimental difficulties involve in determining surface energies of materials.

SVR is a tool in the field of machine learning in which unknown targets are estimated through inference from pattern acquisition. This computational intelligence technique has proved successful in estimating many properties of materials [13–16]. It has been proved as an excellent tool in estimating atomic radii of elements [17] as well as compressive strength of concrete which helps in preventing structural collapse. These achievements of SVR in several fields of studies coupled with the need to circumvent the experimental difficulties in estimating surface energies of materials, serve as motivations for carrying out this research work.

Among the uniqueness of this research work is that it employs a technique that accommodates few experimental data in making excellent generalization. This is a great achievement in the field of surface science where experimental data is limited. Our developed model generated pattern from fourteen experimental data of body centered cubic (BCC) and face centered cubic (FCC) metals and explore the acquired pattern to estimate more than twenty surface energies of HCP metals with high degree of accuracy. This indicates that the model estimates surface energy of materials irrespective of the crystal structure of material used in building the model. Although, there are established connections between HCP and FCC metals (in terms of their crystal structures) which further enhance the predictive and generalization ability of our proposed SVR-based model. Both FCC and HCP crystal structures have closely packed planes of atoms, coordination number of twelve and packing factor of 0.74. The difference comes in their stacking sequence.

During the course of developing the model, our empirical results through simulation indicate 99.08% accuracy for the trained model on the basis of correlation coefficient and improved accuracy of 100% while validating the trained model. This shows the strength of the adopted test-set-cross validation technique of optimization among the pool of optimization algorithms found in literatures [18–20]. The obtained high accuracy further enhances perfect estimation of surface energies of HCP metals when their descriptors are fed into the model.

The remaining part of this work is organized as follows. Section 2 contains brief description of some existing theoretical models, the proposed machine learning technique (i.e. SVR), working principles of the proposed model and the physical explanation of the chosen descriptors. Section 3 explains empirical studies that include dataset description, computational methodology and the employed optimization strategy. Section 4 presents and discuses results while Section 5 entails the conclusion and recommendation.

2. Brief description of the some existing theoretical models

Surface energy is generally referred to as the excess energy at the surface of materials which helps one surface to adhere to another. This excess energy comes from the difference in the energy of the atoms at the surface and at the bulk region of the crystal. Among the models that have been extensively deployed in calculating properties of materials include broken-bond models which approximate to the first-nearest–neighbor interaction and can be further extended to second-nearest–neighbor interaction when better accuracy is desired [21]. It estimates surface energy of materials on the basis of the number of broken bonds [22]. The number of broken-bonds at the surface of materials is known to be proportional to surface energy and this makes closed-packed surfaces to be more stable than open ones. This effect is manifested in the equilibrium crystal shapes of metals with the exposure of closed-packed surfaces at the expense of open ones. Relatively perfect correlation exists between relative surface energies (of different crystal facets) and the number of broken bonds in many FCC metals [23]. Meanwhile, recent review on theoretical models shows that the models that are dominant in calculating surface energies of metals include embedded atomic method (EAM) and equivalent crystal theory (ECT) [5] which was further extended to analytical equivalent crystal theory (AECT) in order to cater for the major challenge that arises in finding the root of ECT equations. EAM is a semi-empirical method that is usually based on approximations to nearest neighbors. It is basically governed by the ideas of density functional theory and is capable of estimating the total energy of a set of atoms in a system by summing the screened coulomb interaction and embedding energy [24]. Embedding energy is obtained when each atom involved in coulomb interaction is inserted in the electron density from all other atoms. The method premises on the fact that the embedding energy is uniquely dependent on the electron density and not on the source while electron density at any site is usually assumed as a linear superposition of spherically symmetric electron densities from other contributing atoms. Due to inefficiency of EAM to generalize well, modification that takes energy change (which arises as a result of non-spherical distribution of electron p_i and deviation from the linear superposition of atomic electronic density) into consideration evolved afterwards.

2.1. Proposed method

SVR is an extension of support vector machines which were mainly developed to tackle classification problems. It employs statistical learning theory and structural risk minimization principle [25–27]. The goal of support vector regression algorithm is to fit a function (which is capable of being used in future to infer output data point that are not previously employed by the function) that approximates the inherited relation which exist between the training dataset (y_i, where $i = 1, 2, 3, \ldots, n$) and the target t_i. The formulation proposed by Vapnik [26] uses ε -insensitive loss function as defined in Eq. (1) as a guide in generating a flat function g that estimates the target in such a way that the incurred error between the target and the output of the function does not exceed ε.

$$\Gamma(t, g(y)) = \begin{cases} 0 & \text{if } \left|t - f(y)\right| \le \varepsilon \\ \left|t - f(y)\right| - \varepsilon & \text{otherwise} \end{cases} \quad (1)$$

A case of linear function g of a form presented in Eq. (2) is described as a complex optimization problem in such a way that minimization of norms $\frac{1}{2}\|w\|^2$ is ensured purposely to have a flat function.

$$f(y) = w \cdot y + b \quad (2)$$

$w \in Y$(input space), $b \in R$ and $w \cdot y$ represents a dot product.

The convex optimization problem illustrated by Eq. (3) is subject to the assumption entails in Eq. (4) which indicates the feasibility of the function.

$$\frac{1}{2}\|w\|^2 \quad (3)$$

Subject to

$$\begin{cases} t_i - (w \cdot y + b) \le \varepsilon \\ (w \cdot y + b) - t_i \le \varepsilon \end{cases} \quad (4)$$

Slack variables $\left(\xi \text{ and } \xi'\right)$ are often adopted so as to accommodate any constraint that can impede the feasibility of the function g. The formulation is therefore stated as

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\left(\xi_i + \xi_i'\right) \quad (5)$$