Application of Data Science on Mechanical Properties of Crystalline materials

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Abstract This study presents a combination of machine-learned models that predicts the surface elastic properties of general free surfaces in face-centered cubic (FCC) metals. These models are built by combining a semi-analytical method [1] based on atomistic simulations to calculate surface properties with artificial neural network (ANN) [2] or boosted regression tree models (BRT) [3]. The latter are also used to link bulk properties and surface orientation to surface properties. The surface elastic properties are represented by their invariants considering plane elasticity within a polar method [4]. The values of these invariants are firstly given in 3D representations with surface orientation variations, which clearly demonstrate anisotropic behaviors, see Fig. 1(a). The forms of these invariants in the 3D representation are relatively similar among the different pure metals considered, but with different magnitudes. Furthermore, it is found that the spherical part of the residual surface stress tensor is always positive, which means the free surface is always in a tensile state. The developed models are shown to accurately predict the surface elastic properties of seven pure FCC metals (Cu, Ni, Ag, Au, Al, Pd, Pt), see Fig. 1(b). The BRT model reveals the correlations between bulk and corresponding surface properties in terms of invariants (Fig. 1(c)), which can be used to guide the design of complex nano-sized particles, wires and films. Finally, these model constructs enable us to express the surface excess energy density as a function of surface elastic invariants for quick predictions of surface energy as a function of in-plane deformations.

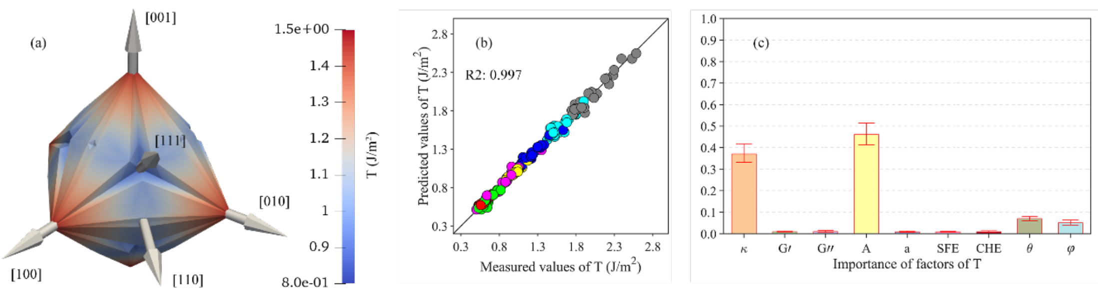

Figure 1 - *(a) 3D representation of the spherical part of the residual surface stress tensor (T) for Cu free surfaces, (b) cross-validated predictions vs. calculated results of T with error scores (the 7 different colors correspond to the 7 studied metals), and (c) analysis of the importance of the input*

factors used in BRT for the prediction of T. κ is the bulk modulus, G' the {001} <110> shear resistance, G'' the {001} <100> shear resistance, A the elastic anisotropy ratio, a the lattice parameter, SFE the stacking fault energy, CHE the cohesive energy and θ and φ spherical coordinates to represent the surface orientation.

Keywords:

Surface elastic invariants *Molecular statics* *Machine learning*

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