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Elastic model of BCC high entropy alloys.

Bassem Sboui [a b], David Rodney [a], Pierre-Antoine Geslin [b]

[a] *Institut Lumière Matière - Université Claude Bernard Lyon 1, 69622 Villeurbanne, France*

[b] *Laboratoire MATEIS - INSA Lyon, 69621 Villeurbanne, France*

[a] *bassem.sboui@insa-lyon.fr*

High entropy alloys made of refractory elements and presenting a single BCC phase conserve exceptional mechanical properties at elevated temperatures [1]. Nevertheless, their plastic behavior is not yet fully understood as a function of their composition and their interstitial content.

The objective of this work is to study dislocation-mediated plasticity in HEA with a BCC structure (e.g. Ta25Nb25Mo25W25) by means of a continuous elastic model carefully parametrized from atomistic calculations.

Based on previous contributions [2,3], we first develop an elastic model of BCC HEAs that considers each atom as an Eshelby inclusion embedded in a continuous framework. The mean-square displacement predicted by the elastic model can be compared to atomistic simulations. If a unique diagonal eigenstrain tensor (i.e. a unique misfit volume) is considered for each element, the elastic model underestimates significantly the mean square displacement. We show that the discrepancy can be corrected by considering an environment-dependent anisotropic eigenstrain tensor. The methodology to compute the atomic eigenstrain tensor will be presented. In a second step, we use this elastic framework to compute the variance and spatial correlations of shear stresses that control dislocation motion and therefore the yield stress of the alloy.

Keywords: High Entropy alloys, Microelasticity theory.

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