

Abstract Submitted  
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**Multiscale model for the study of phase separation in alloys with elastic misfit**<sup>1</sup> DANNY PEREZ, LAURENT LEWIS, Université de Montréal — We present a multiscale model developed for the study of phase separation and microstructure evolution in binary alloys. The model is based on the classical time-dependent DFT formalism for lattice systems generalized so that elastic effects are taken into account. A multi-scale implementation of this formalism is then performed using the finite volume method to obtain the evolution of the diffusive degrees of freedom while the quasicontinuum method is used to relax the elastic degrees of freedom. The combination of these two methods allows for a seamless coupling between different length-scales using a single formalism, while reducing exactly to the original TDDFT model as the mesh size is reduced to atomic dimensions. As a first application of this model, we study the effect of elastic heterogeneity on the chemical potential of inclusions as a result of inclusion-matrix and inclusion-inclusion interactions, and infer the consequences on the coarsening behaviour of a collection of inclusions.

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