ON-LATTICE MODELS TO STUDY EVOLUTION OF HEA AT ATOMIC SCALE

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High-entropy alloys (HEA) is a new perspective class of metallic materials. These alloys contain at least four principle elements in approximately equal concentrations. HEAs with outstanding properties have already been discovered. For instance, some of the alloys have excellent mechanical properties at elevated temperatures; others demonstrate good corrosion resistance, and even enhanced radiation tolerance.

However, these effects remain unexplained, since simulation of HEAs at atomic scale is hindered by complex chemical composition of the material. In particular, quantum molecular dynamics (MD) could not reach required time- and space-scales, while classical MD does not provide sufficient accuracy. Therefore, a new approach is needed, which will be capable of accurate and yet computationally feasible description of HEAs at atomic scale.

Such approach is proposed in this work. We describe evolution of a HEA in the framework of kinetic Monte-Carlo, coupled to on-lattice interatomic potential [1]. The model reproduces the results of quantum-mechanical calculations with error less than 5 meV/atom. The proposed approach allows to reveal ordering of FeCoNiCr, and formation of Fe and Cr super-lattices.

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1. Shapeev A. // Computational Materials Science. 2017. V. 139. P. 26