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Atomic displacements in binary alloys YEVGENIY PUZYREV, Oak Ridge National Laboratory, J.S. FAULKNER, Florida Atlantic University, G. E. ICE, C.J. SPARKS, Oak Ridge National Laboratory — Molecular dynamics calculations are used to model the thermal and static displacements in copper and copper-gold alloys. Adjusted embedded atom potentials that give very accurate atomic sizes for the pure metals are used. The agreement with experiments supports the argument that this is a reliable approach for predicting displacements, and will be useful in interpreting experimental data on atomic displacements in metals and alloys. The positions of the atoms in a binary alloy at temperature T at all times t,$\mathbf{R}_i(t)$, can be found using molecular dynamics (MD)[1] if the forces on the atoms are known. It is still necessary to use supercells, but they can contain thousands of atoms. The set of $\mathbf{R}_i(t)$ contains all the information about both static and thermal displacements. Of course, MD is a classical theory, and the only quantum mechanical effects appear in the construction of the forces.

[1]D. C. Rapaport, *The Art of Molecular Dynamics Simulation*, **2**nd edition (Cambridge University Press, Cambridge, U. K., 2004)

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