Comprehensive model of metadislocation motion in o-$Al_{13}Co_4$

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In several complex metallic alloys plastic deformation is mediated by metadislocations. Due to the complex nature of these defects and the large number of atoms in their core region, little is known about the atomic rearrangements taking place during movement of a metadislocation. Up to now, available models have been limited to two dimensions and heavy elements.

In this work we report on the first development of a fully three-dimensional model of a moving metadislocation including all atomic species. The CMA chosen for our study is the moderately complex o-$Al_{13}Co_4$, an orthorhombic phase with space group $Pmn2_1$, lattice parameters a = 8.2 Å, b = 12.3 Å , c = 14.5 Å and 102 atoms per unit cell.

Using a combination of high-resolution scanning transmission electron microscopy and density functional theory, we have developed an atomic model for the [010] glide movement of a metadislocation in $Al_{13}Co_4$ extending to light elements and including the third dimension. Metadislocation movement was analysed employing a simulated-annealing procedure to minimize the total jump distance of all atoms within the model. The results of different simulated-annealing runs typically deviate in the range of 0.5% with respect to the total jump distance, due to slight local differences in the jump scheme of aluminium atoms. While the distance of one glide step is 12.3 Å , the maximum jump distance of an individual atom is a much more moderate 3.4 Å . The approach described is versatile enough to be applied to other, more complex problems, for example metadislocation movement in □$_6$-Al-Pd-Mn.

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[1] M. Heggen and M. Feuerbacher, “Core structure and motion of metadislocations in the orthorhombic structurally complex alloy Al13Co4,” Materials Research Letters 2, 146–151 (2014).