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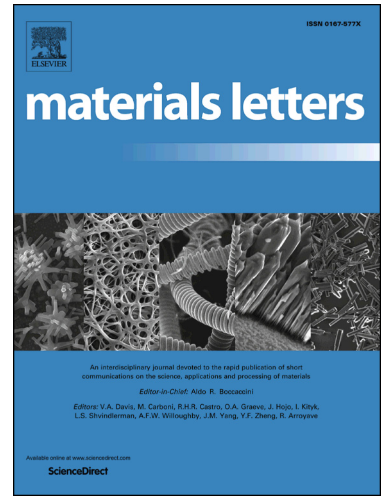

Modification of dislocation emission sources at symmetric tilt grain boundaries in Ag by Cu solute atoms

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Modification of dislocation emission sources at symmetric tilt grain boundaries in Ag by Cu solute atoms

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Abstract

A very small amount of immiscible solutes can dramatically decrease the ability of dislocations to nucleate from grain boundaries. In this this paper we report the results of the molecular dynamics simulations which show that at larger concentrations, the solute effect becomes rather non-trivial: there are concentration ranges where even small addition of solutes considerably suppress the dislocation nucleation from grain boundaries and there are concentration ranges where addition of new solutes almost does not change the dislocation nucleation ability. We reveal the atomic mechanism of these effects.

Keywords: solute segregation at grain boundaries; dislocation emission source; yield stress; Monte Carlo simulation; molecular dynamics simulation.

1. Introduction

The grain size of polycrystalline materials strongly affects the plastic deformation behavior [1]. In particular, it is well established that a significant strengthening can be achieved with decreasing grain size [2]. However, if the grain size is very small (<15 nm) a softening can happen due to the crossover from the dislocation-mediated plasticity to the grain boundary (GB) mediated plasticity [3,4]. The thermal instability of most nanocrystalline materials represents another problem for their commercial applications. This instability is associated with the significant grain growth/coarsening which can occur at relatively low temperatures. The addition of immiscible solutes, which tend to segregate at grain boundaries, can be a solution to both problems mentioned above. On one hand, solutes segregated at GBs can stabilize nanocrystalline material against grain growth [5-7]. On the other hand, they can suppress GB mediated plasticity mechanisms [8]. Keeping in mind that dislocation emission from grain boundaries is a key deformation mechanism for a wide range of grain sizes [9,10], it would be ideal, if the solutes added in order to stabilize the material against the grain growth and GB sliding/rotation, would also suppress the nucleation of the dislocations from the same grain boundaries. Using molecular dynamics (MD) simulation, we demonstrated that solutes can indeed have a very strong effect on the process of the dislocation emission from GBs [11]. This effect is very strong at small concentrations but levels off at larger concentrations. While the origin of the solute effect on the dislocation nucleation at small solute concentrations was discussed in details in [11], the reason for leveling off at larger concentrations was not considered. In the present paper, we report additional data points obtained for larger concentrations and discuss the mechanism of the solute