

Uncovering the role of solute-trapped vacancies on precipitation pathways in Al-Cu-In-Sb alloy

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Light weight alloys have been widely used in automotive and aerospace industries, where fuel economy is a main concern. Al alloys which can be hardened by nano-scale precipitates are presently main candidates or players. The study on the precipitation mechanism traces back to 100-year ago [1]. However, until now, we cannot design the mechanical properties on demand by optimizing the characters of nano-scale precipitates. An alloy with excellent mechanical properties are still products of trial and error [2], though the Materials Genome Initiative and atomic resolution characterization have been there for several years [3]. One limitation is kinetics are often absent in computer simulations. Here, we show how diffusion kinetics change the precipitation pathways in an Al-1.7Cu-0.025In-0.025Sb (at. %) alloy [4].

Fig. 1 shows InSb truncated octahedron forms first and then promotes the heterogeneous nucleation of GP zones, θ'' and θ' consequently. The moiré fringe and nano diffraction pattern of the InSb particles suggest In and Sb atoms stack in FCC lattice but with a large lattice parameter ($a=0.48\text{nm}$) than Al matrix. The large lattice mismatching (18%) between InSb and θ' makes the heterogeneous nucleation different from common observation: here structural reconstructions occur between the two phases, as shown in Fig. 2 a. There is also a minor precipitation sequence, where θ' form first and then InSb (Fig. 2 b).

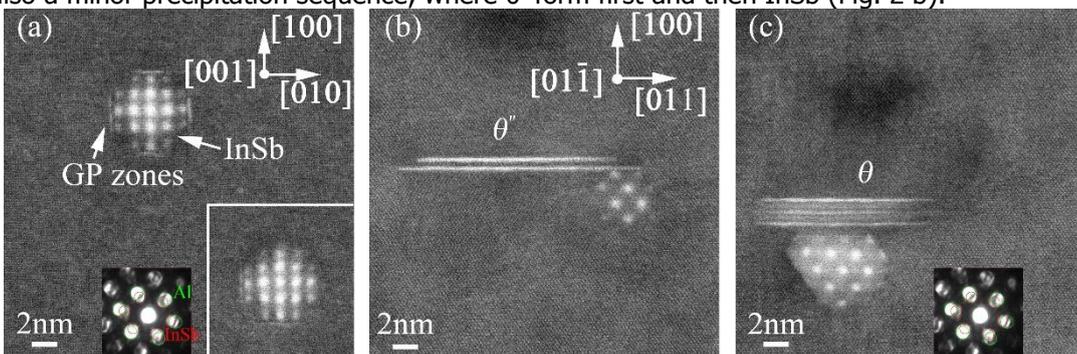


Fig. 1 HAADF images of the alloys aged at 200 C. (a) 2min, the inset is an InSb particle truncated only at two faces, (b) 10min, (c) 10min. Nano diffraction pattern of the InSb particles are also shown as insets.

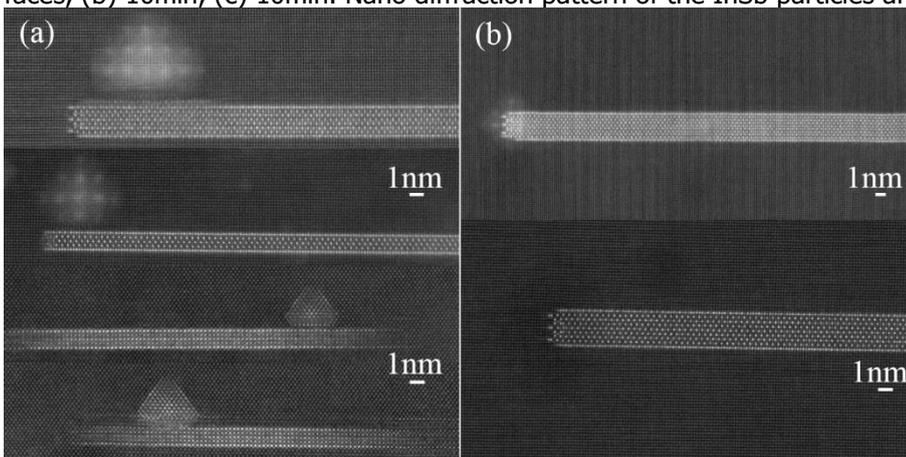


Fig. 2 HAADF images for the alloy aged for 30 min at 200 C.

Fig. 3 shows the minor pathway becomes the dominant one at high ageing temperature. Therefore, the precipitation pathways seem to depend on temperature which can affect both kinetics and thermodynamics. However, we also succeed in reversing the precipitation sequence, i.e., making the sequence independent of ageing temperature and excluding the thermodynamics role. Binding energies between vacancies and In and Sb calculated from density functional theory (DFT) suggest excess vacancies escaped from In and Sb traps accelerate the diffusion of Cu and change the precipitation sequence.

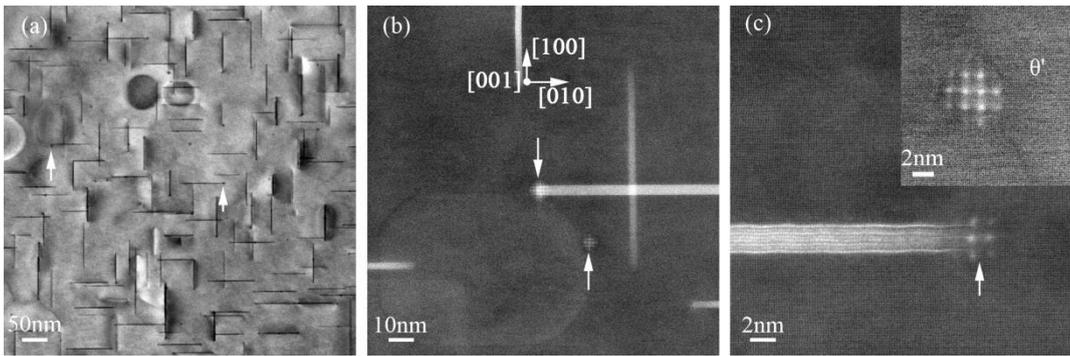


Fig 3. Images of the alloy aged at 250 C for 2 min: (a) BF image, (b) and (c) HAADF images, arrows indicating InSb particles.

References

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