Mode II loading behaviour of intergranular nanocracks lying on a $\Sigma17(530)$ symmetrical tilt boundary in copper

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Recently the phenomenon of the grain boundary (GB) movement as a consequence of applied mechanical load has attracted much attention [1–4]. Shear-coupled migration (SCM) of tilt boundaries has been acknowledged as a particular plastic strain mechanism that can complement or compete with the other intra– or inter–granular mechanisms in a wide temperature range. SCM is diffusion–less but thermally activated. The shear strain effectiveness of the migration of a tilt boundary can be characterized by a shear coupling factor, β, the ratio of the shear displacement parallel to the GB surface to the GB migration normal to its surface. The factor β is determined by the tilt GB misorientation, θ, either $\beta = 2\ \mathrm{tg}(\theta/2)$ ("small" misorientations) or $\beta = -2\ \mathrm{tg}(\varphi/2)$, $\varphi = \pi/2 - \theta$ ("large" misorientations).

In this work MD simulations of SCM of a $\Sigma17(530)/[001]$ symmetrical tilt boundary ($\theta = 61.9^\circ$, $\beta = -0.5$) in copper have been carried out aiming to compare the behaviour of a perfect boundary with that of a boundary containing nanocracks lying on its surface. Details of the MD technique, the Embedded Atom Method and the copper potential employed in the simulations are given elsewhere [5]. The Nosé-Hoover thermostat [6] was implemented for temperature control. Simulations have been carried out at $T = 300$ K using time increments $\Delta t = 2.5\times10^{-15}$ s.

Prior to sample virtual testing, the cracked or uncracked bicrystals of $14.8\times2.2\times21.0\ \mathrm{nm}^3$ of size were constructed at 0 K, the cracks being formed by removing the atoms located in a band of 0.55 nm centred in the GB along 1/3 of the specimen size in the x direction. They were relaxed during 5 ps at 0 K and during 12.5 ps at 300 K under no constraints, for the GB to acquire its metastable configuration. Surface tension leads to some global and geometrical distortion of the initial shape of the bicrystals. In all of the tested cases, the $\Sigma17(530)$ symmetrical tilt boundary showed negative shear coupling, in agreement with the reported negative coupling for $\theta \geq 35^\circ$ in [001] tilt boundaries [3]. After relaxation, two rigid zones 0.55 nm thick were established in the upper and lower layers of the samples. During the virtual shear test, the lower rigid zone remained fixed, the upper part being displaced at a constant rate of $2.12\ \mathrm{m\cdot s^{-1}}$ ($\dot{\gamma} \approx 10^8\ \mathrm{s^{-1}}$). Periodic boundary conditions were set along the x and y axes.

Figure 1 shows the nominal shear stress, τ_{nom}, as a function of the nominal shear strain, γ_{nom}. The average shear stress in the ligament of the cracked specimens is 1.5 times higher than that value. For the uncracked tilt boundary the result reproduces the behaviour observed at similar homologous temperature by other authors [3, 4], characterized by a stick–slip phenomenon associated to the GB migration when certain shear stress (≈ 0.3 GPa) is overcome. The slopes of the intermittent elastic loading stages are 27 GPa. The presence of a crack affects the mechanical response of the samples. The cracked specimen shows similar stick–slip behaviour but the shear stress increases monotonically with strain till a value of 1.5 GPa at $\gamma_{\mathrm{nom}} \approx 0.12$, when a sudden drop of the stress occurs.

The bicrystal is thus strengthened by the presence of intergranular cracks. The situation is similar to the strengthening of a crystal by a dispersion of nanovoids in dislocation-mediated plasticity. The shear strain–induced structural changes explain this anomalous behaviour (Fig. 2). Although the crack strongly amplifies the shear stress in the vicinity of the tip, the GB of the cracked bicrystal is pinned by the crack. SCM occurs away from the crack tip, the GB bowing out (downwards as $\beta < 0$). The shear stress applied on the GB surface close to the crack tip weakens because of the progressive GB misorientation. Migration of the GB progressively becomes more difficult until GB depinning from the crack (small $|\beta|$) helped by partial dislocation emission from the crack tip.

Acknowledgements

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Figures

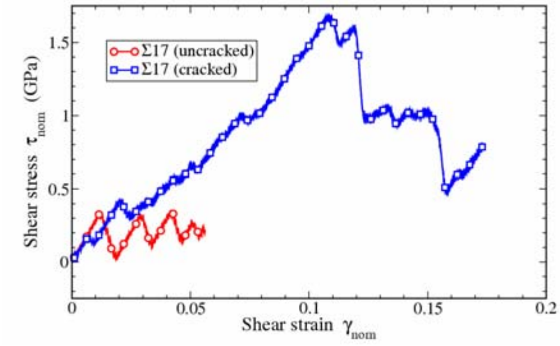
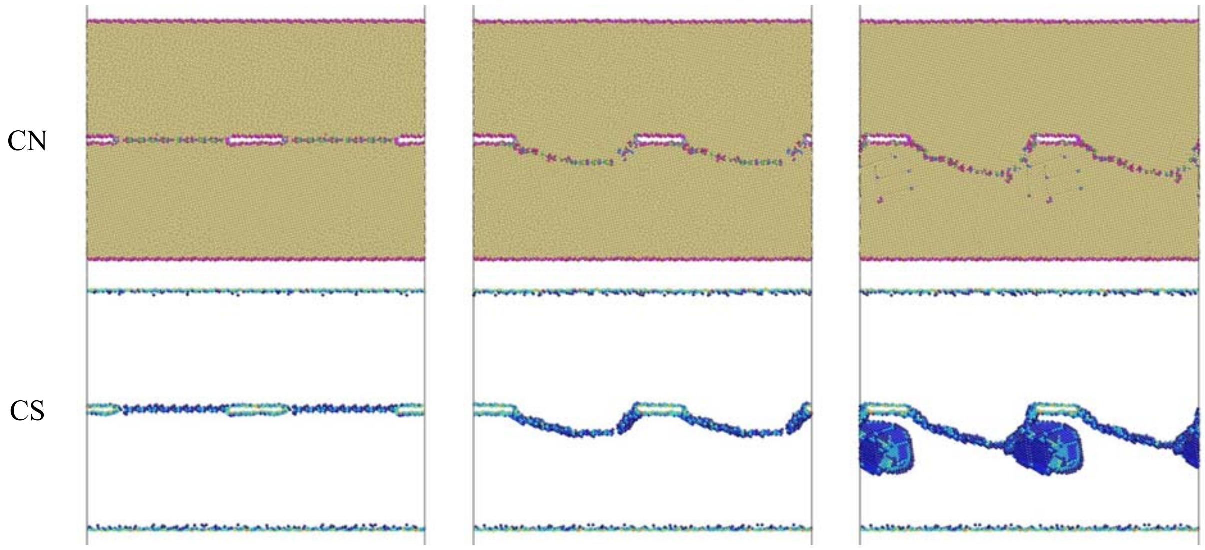


Figure 1. Nominal shear stress, τ_{nom}, vs. nominal shear strain, γ_{nom}, curves of the un-cracked and the cracked bicrystals of the Σ17(530) symmetrical tilt boundary.



(a) (b) (c)

Figure 2. Copper bicrystal (Σ17(530)/[001] tilt boundary) under imposed shear displacement parallel to the boundary plane. The tilt axis is perpendicular to the figure. The bicrystal contains periodically spaced through–thickness intergranular cracks. Images are snapshots at macroscopic strain (a) $\gamma_{nom} = 0$,

(b) $\gamma_{nom} = 0.08$ and (c) $\gamma_{nom} = 0.12$. Depinning of the GB occurs shortly after that strain. Coordination number (CN) makes visible the GB and partial dislocations, centro-symmetry (CS), the stacking faults.