Effect of θ' hybridization on shear strength of Al-Cu alloys: multiscale study

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We use a multiscale approach, combining molecular dynamics (MD), continual modeling and discrete dislocation dynamics (DDD), to determine the effect of precipitate hybridization on macroscopic strengthening in Al-Cu alloy. We perform MD calculations of the dislocation motion in aluminum containing strengthening phases. The work considers two types of hardening inclusions, the structure of which was recorded in [1] by electron microscopy. The first type of inclusion is θ' phase, the second type is hybrid inclusion, which has a sandwich structure with a tetragonal θ' lattice in the core and GP-like structures along the broad interfaces. MD simulations evidence a complex dislocation precipitate interaction mechanism, including bending of both hybrid and non-hybrid precipitates at the early stages of interaction, deformation and cutting during multiple passage of a dislocation. MD results are used to calibrate a continuum model proposed in [2]. We use method of discrete dislocation dynamics, in which a computational domain, containing a large number of dislocations and hardening inclusions is considered. It was found the shear strength of alloy with hybrid precipitates to be 20% higher than that for non-hybrid plates at the same copper content of more than 2 wt.%.

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[1] Bourgeois L, Zhang Y, Zhang Z, Chen Y and Medhekar N V 2020 *Nat. Commun.* **11** 1–10

[2] Krasnikov V S, Mayer A E, Pogorelko V V, Latypov F T and Ebel A A 2020 *Int. J. Plast.* **125** 169–190