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# Séminaire

SRMP

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**Salle de réunion du SRMP – Bâtiment 520 - Pièce 109**

# *Influence of the substitutional elements on the <a> type screw dislocation glide in α-Ti - solution strengthening vs ductility enhancement*


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The mechanical properties of hexagonal Ti alloys depend substantially on the glide of <*a*> type screw dislocations. The configurations and stabilities of these line defects are, however, known only in pure Ti and Ti + O solutions, where the locking-unlocking mechanism [1,2] and a strong pinning effect [3] control their activity. In this study, we investigated the unclear, screw dislocation mediated solution strengthening of substitutional α-Ti alloys. To this end, a first principle computational scheme was used to determine the structures and energies of the considered line defects during planar and cross-slip processes in the vicinity of the solute element. Special attention was paid to analyze the basal screw dislocation core spreading and glide which is known to be unstable in pure Ti improving anisotropy of plasticity and limiting ductility of the material. The determined interaction energies between substitutional solutes and <*a*> type screw dislocations are relatively large even a few times greater than Peierls barrier of high energy pyramidal glide in pure α-Ti–which shows the significant impact of substitutional solutes on screw dislocation mobility. Moreover, transition metals reduce the energy of the considered line defects, stabilizing its position and impeding further glide. Simple metals also introduce high energy dislocation states (dislocation repulsion) which improves the overall solution strengthening effect. The observed enhancement of screw dislocation core polymorphism leads to their new configurations unavailable in pure α-Ti, like high energy basal spreading activated by simple metals. The calculations performed also indicate In as a potential alloy element for improving both the strength and ductility of Ti by stabilizing a special, compact core geometry able to spread on an arbitrary glide plane with a low energy barrier. All of the above effects are discussed in terms of the physical factors (solute size misfit, stacking fault energy and electronic structure) that affect the energy and geometry of dislocation cores [4,5].


**References:**


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