SOLID SOLUTION STRENGTHENING OF HEXAGONAL TI ALLOYS: STRUCTURES, ENERGIES AND PEIERLS BARRIERS OF <A> TYPE SCREW DISLOCATIONS CALCULATED FROM FIRST PRINCIPLES

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1. Introduction

Due to their finely balanced strength and density, hexagonal close-packed (hcp) metals such as Ti and Mg are perceived as potential prime elements for the production of new light, and strong alloys essential for the sustainable development of green technologies oriented towards a reduction in mass in all transport sectors. Nevertheless, the conscious design of materials requires information on the relationship between alloy elements and individual deformation mode activity. Such complex knowledge in the context of hcp systems remains a challenge, seriously hampering our ability to anticipate the strength and ductility of new materials developed. In general, hcp metals and alloys suffer from limited cold workability arising from reduced crystal symmetry (compared to cubic crystals) and from the geometrical relations between their dislocation glide planes [1]. On the other hand, the unique properties of single phase hcp materials, such as great strength and reasonable ductility of α-Ti+O solutions [2,3] and a pronounced solution softening of α-Mg+Y alloys [4,5], demonstrate the great potential of this groups of materials. All these aspects provide incentive for exploring the physics of plastic deformation and solution strengthening theories.

2. General

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 [6] and Ti + O solutions [7], where the locking-unlocking mechanism and a strong pinning effect 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. Two phenomena were determined that are crucial in terms of plastic deformation: (i) enhanced polymorphism of the dislocation cores leading to multiple new core configurations, and (ii) relatively large positive and negative interaction energies between the solutes and the line defects. Both these effects are strongly affected by the valence configuration of the alloying elements. Due to their pronounced structure and energy variations, dislocation planar and cross slip processes can occur under different scenarios, through diverse non-planar core geometries. 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.

3. Graphical presentation of computational results

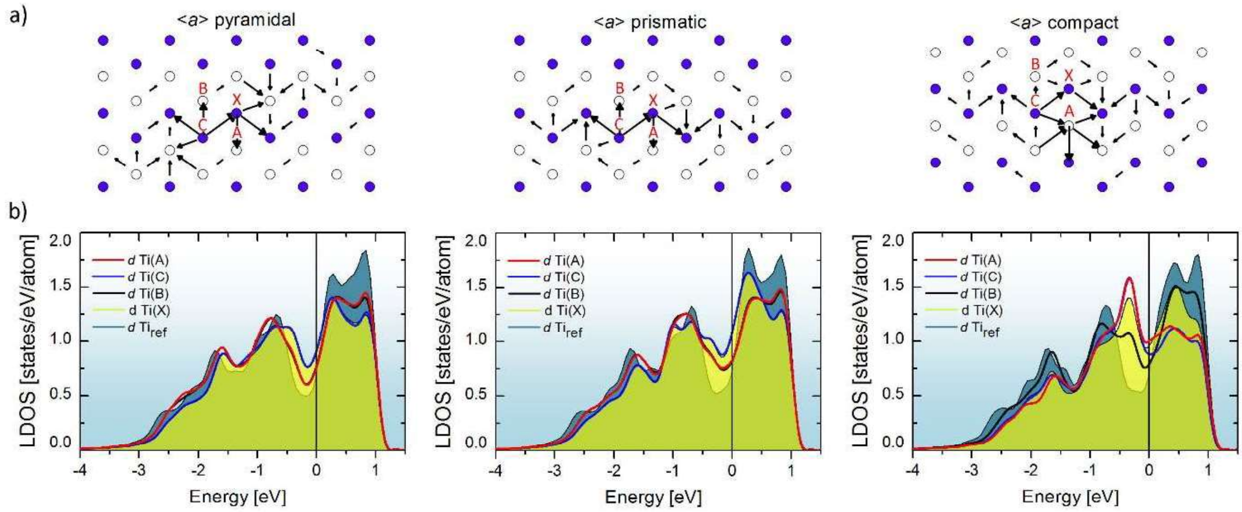

Fig. 1. Detailed structures of selected <a> type screw dislocation cores (a) and local density of states plots determined for X, C, B and A atomic position (b) [8]

4. Conclusions

This article describes the impact of substitutional solutes on α-Ti screw dislocation geometry, energy and motion. The alloying elements used in this study belong to two groups: simple (Sn, Ga, In) and transition (V, Zr) metals; this makes it possible to study the effect of solute valence structure on line defect behaviour. All calculations were performed within an ab initio framework, utilizing the full periodic boundary condition approach of dislocation modelling. The determined interaction energies between the substitutional solutes and <a> type screw dislocations are relatively large, even a few times greater than the 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.

5. References

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