STACKING FAULTS IN HEXAGONAL TI ALLOYS – LOCAL INSTABILITY OF CRYSTAL LATTICE AND ITS EFFECT ON SOLUTION STRENGTHENING

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1. Introduction

Stacking faults are the special regions of the crystal structure that exhibit non-uniform structure and diversified stability. Energy of this defects determines configurations of dislocation cores and type of predominant plastic deformation mechanism. In this study we focus on the generalised stacking fault energy computations of multi-slip-system hexagonal Ti alloys in the context of solution strengthening effect and the atomic as well as electronic structure identification of the analysed planar defects.The far reaching goal is to provide the physical basis and theoretical infrastructure to answer the still unresolved question concerning the initiation of a micro-shear band in metallic solids.

2. General

The solid solution strengthening of α-Ti was investigated in respect of dislocation nucleation and dissociation in all four active glide modes. A series of Ti+X alloys (X = Al, Sn, V, Zr and O) was selected to analyse the impact of solute valence structure (Al, Sn - p type elements, V, Zr - d type elements) and lattice site (interstitial O) on the mechanisms responsible for variation of mechanical properties. The computational procedure relied on the generalized stacking fault energy (GSFE) concept combined with the nudged elastic band method that enables full atomic relaxation and determination of the true, minimum energy GSFE path [1]. Additionally, various concentrations of solutes and their distance to the glide plane were considered as well. Our study revealed a strong, nonlinear influence of X position on GSFE and migration of O atoms during the crystal slip. These new phenomena allowed one to determine three solution strengthening mechanisms:

(I) hindrance of <a> prismatic dislocation emission and reconfiguration of 1/3 <1120> screw dislocation cores (p type solutes),

(II) hindrance of <a> prismatic dislocation emission (V) and SFE reduction in other modes (both d type solutes),

(III) suppression of dislocation nucleation in all modes caused by O [2,3,4].

We found that the stacking faults formed by the single partial dislocations have a thickness of few atomic layers and exhibit a highly non-uniform structure. Their ability to accommodate the lattice deformation introduced by solute elements greatly affects the stacking fault energies of the α-Ti alloys.

3. Graphical presentation of computational results

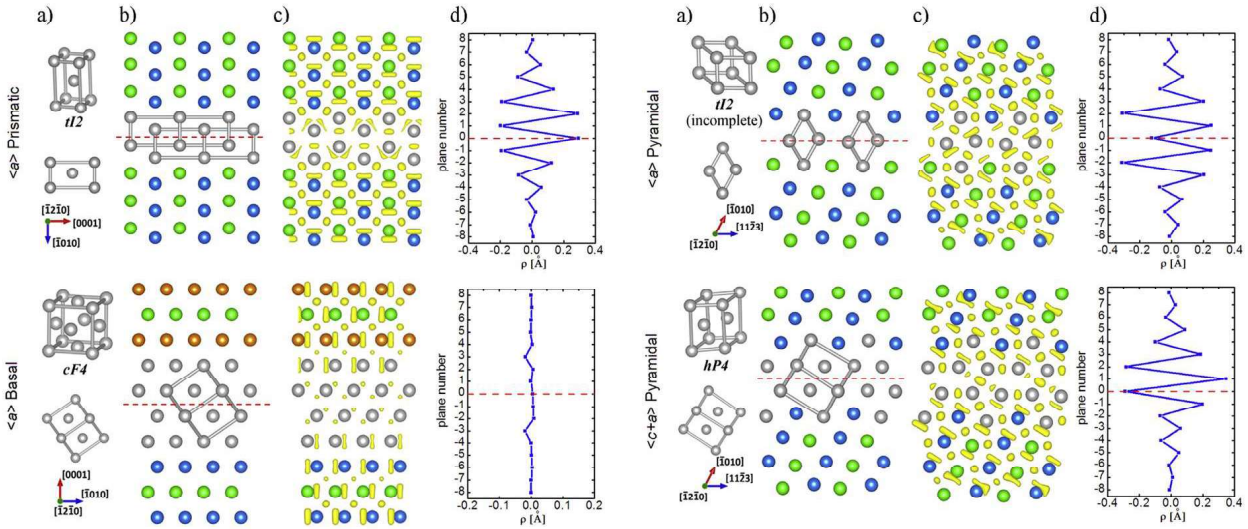

Fig. 1. Hexagonal Ti stacking faults: unit cell, Pearson number and orientation relative to host crystal (a), SFs structure arrangement (b), atomic bond patterns (yellow zones indicate electron-localization-function ELF isosurfaces) (c) and interplanar distance distortion plots (d). The gray spheres depict atoms belonging to SF regions while blue, green and orange ones denote A, B and C sequence of basal planes in unaltered sections of the crystal. Slip planes are marked by the red dashed lines. The ELF isosurface level is equal to 0.7 in all cases [5].

4. Conclusions

Conclusion of this study can be useful not only in terms of analysis of the line defects core geometries but also for phenomena influencing instability of plastic deformation i.e. nucleation and configuration of slip bands boundaries. The understanding of slip phenomena that appear in the active zone of initiating and propagating micro-shear band can be helpful in the formulation of theoretical description of plastic deformation accounting for multiscale shear banding processes [6].

5. References

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