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Tunable twin stability and an accurate magnesium interatomic potential for dislocation-twin interactions☆

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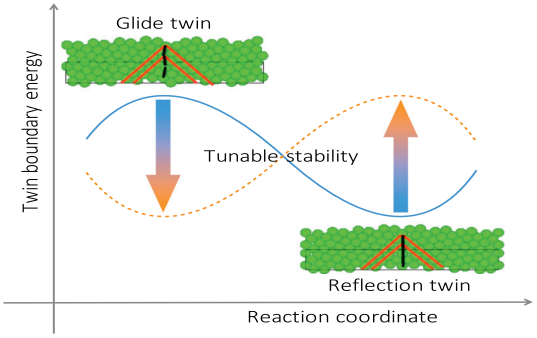
HIGHLIGHTS

- We find the stability of two variants of twins is reversible and tunable, which is controlled by twin boundary energies.
- The tunability represents a potential pathway to design novel Mg alloys with tailored mechanical properties.
- A comprehensively optimized potential is developed for Mg that incorporates information of dislocations and twins.
- The new potential will provide new momentum to the studies of complex defect-defect interactions in Mg.

GRAPHICAL ABSTRACT



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ABSTRACT

We showed that there are two variants of twin boundaries for each twin system in hexagonal close-packed materials in our previous study. In this work we further demonstrate that the mechanical stability of these two twin variants in Mg are controlled by their energies and theoretically tunable. In the second part of this work, we continue to incorporate this information of twin boundaries into a newly developed embedded-atom-method (EAM) potential for pure Mg. In addition to twins, the other important information of dislocations and stacking faults is also included, which renders our potential among one of the rare comprehensively optimized ones. Therefore our potential is supposed to be able to accurately capture the physics of not only single defect but also defect-defect interactions. The defect-defect interactions have not been adequately addressed, since modeling their long-range force fields based on density functional theory is computationally too expensive. The new potential will supply new momentum to the study of defect-defect (such as twin-dislocation) interactions and the defect-controlled mechanical properties in Mg. Our study therefore sheds light on the design of novel Mg alloys with optimized mechanical properties.

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1. Introduction

Magnesium and its alloys have attracted great attention in the past decades. These materials are very promising next-generation light-weight structural materials due to their high specific strength [1,2]. However, their wide applications are hindered by their low ductility controlled by dislocations and twins [3,4]. The ⟨*a*⟩ slips on basal, prismatic and pyramidal planes and tensile {10$\bar{1}$2} twins are the common deformation modes in hexagonal close-packed Mg and Mg alloys. Understanding the individual defects and the interactions between these defects at the atomic scale is of great significance in the design of ductile Mg. Once the dominant mechanisms of brittleness are clarified we can decide which solutes (making novel Mg alloys) are needed in order to weaken the mechanisms and thus design Mg alloys with better ductility. Atomistic simulations based on embedded atom method (EAM) or modified EAM (MEAM) are practical ways to study these problems since the more accurate density functional theory (DFT) is generally computationally too expensive in dealing with the long-range force fields of these defects.

In previous work, single defects (such as one dislocation or one twin boundary) as well as their interactions with solutes have been extensively investigated [5-10]. On the contrary, the more complicated interactions between different defects (e.g., dislocation-dislocation, twin-twin and twin-dislocation) are less well-understood. Recent studies have started to shed light on the complex defect interactions, both experimentally and theoretically [11-14]. Among the various types of interactions, the basal ⟨*a*⟩ and {10$\bar{1}$2} tensile twin interaction has raised substantial interest because it may account for the nucleation of the non-basal dislocations. Non-basal dislocations (such as {11$\bar{2}$2}⟨11$\bar{2}$3⟩ slip) are able to supply the out-of-basal-plane strain and are deemed as a crucial mechanism for improving the ductility of Mg [4,5,15,16]. In order to simulate the dislocation-twin interactions at the atomic scale, an empirical potential of good quality is much needed.

There are at least 7 versions of EAM/MEAM potentials available in the literature to investigate the mechanical properties of Mg and some of them have been reported to be effective in describing the mechanical properties of Mg. For example, Liu et al. [17] and Sun et al. [18] developed EAM potentials for pure Mg, which are among the most popular potentials. A Mg-Y EAM potential was developed by the authors specifically for the simulation of dislocations [19], followed by Kim et al. who developed MEAM potentials of Mg alloys [20]. Besides, Wu et al. developed a new version of MEAM potential for pure Mg [21] and published their findings of dislocation behaviors employing the potential in [22]. Despite so many EAM or similar potentials published in the past decades for Mg, few of them include the information of both dislocations and twins at the same time. In this study we release an EAM potential for Mg that will exactly fill this gap.

Although the present work is focused on the study of defects in pure Mg, it is highly valuable to the design of ductile Mg alloys. The defects involved in this study (i.e., dislocations, twins and stacking faults) are the key to understand the brittleness of pure Mg. The behavior of these defects individually or collectively leads to a variety of mechanisms that may determine the brittleness of pure Mg. In this study, we not only supplied a highly optimized Mg interatomic potential to investigate these mechanisms but also included exciting results towards this direction.

2. Methodology

2.1. Geometries of slip systems and the tensile twin

In this study, we consider five different slip systems and the most profuse tensile twin boundary for pure Mg. The crystallographic parameters of slip systems (0001)[11$\bar{2}$0], (10$\bar{1}$0)[11$\bar{2}$0], (10$\bar{1}$1)[11$\bar{2}$0], (0001)[10$\bar{1}$0], (11$\bar{2}$2)[11$\bar{2}$3]and the {10$\bar{1}$2} tensile twin are illustrated in Fig. 1. In order to benchmark the EAM potentials, we compare the generalized stacking fault energies (GSFEs) of the five slip systems with the DFT results. Moreover, three gamma surfaces (for the basal, prismatic and pyramidal I planes, respectively)

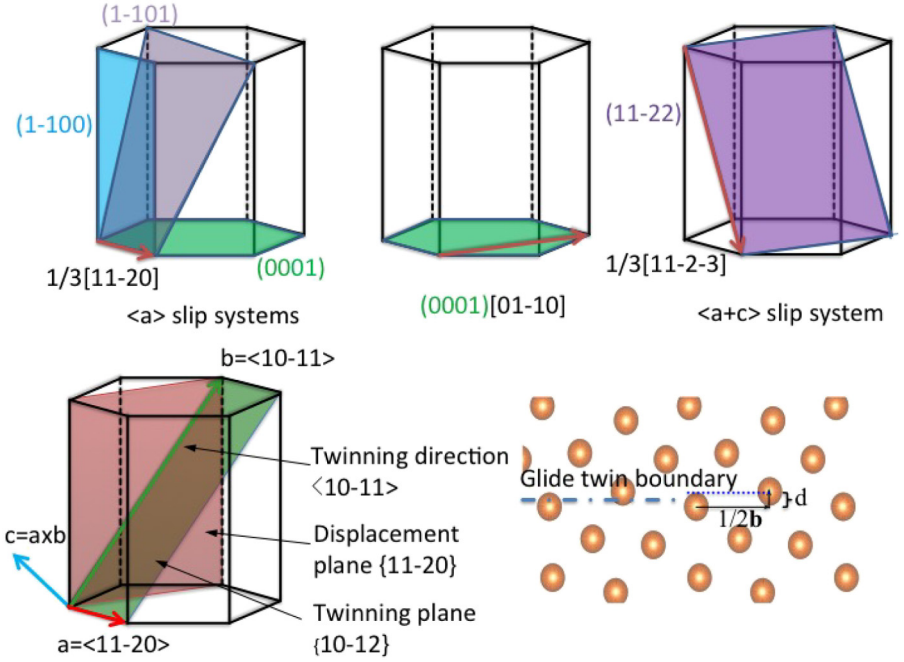

Fig. 1. The schematic of the slip systems and the tensile twin ({10$\bar{1}$2}) for hexagonal close-packed Mg. The characteristic parameters for the tensile twin boundary are illustrated in its glide variant.