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Energy paths of twin-related lattice reorientation in hexagonal metals via *ab initio* calculations

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ABSTRACT

Employing *ab initio* calculations, we systematically investigated the energy paths of $\left[10\bar{1}2\right]$ twin-related lattice reorientation in hexagonal metals Be, Mg, Sc, Ti, Co, Y, Zr, Tc, Ru, Gd, Tb, Dy, Ho, Er, Tm, Lu, Hf, Re, and Os. Among the studied systems, lattice reorientation energy increases in the order of Mg, Gd, Tb, Dy, Zr, Tc, Ti, Ho, Y, Co, Er, Sc, Be, Tm, Lu, Hf, Re, Ru and Os. The reorientation process consists of shear and shuffle components. Concerning the significance of shuffle, these hexagonal metals fall into two groups. In the first group, which includes Mg, Co, Ru, Re and Os, regardless of the shear amount, subsequent shuffle is an energy-uphill process, while in the second group, which includes Ti, Tc, Be, Y, Gd, Tb, Dy, Ho, Zr, Er, Sc, Hf, Lu and Tm, shuffle becomes an energy-downhill process if shear component reaches an adequate level (at least 60%). These results qualitatively explain the present observation of lattice reorientation in hexagonal metals, and shed light upon a general understanding on the $\left[10\bar{1}2\right]$ twinning behavior in the aim of improving materials properties.

1. Introduction

Twinning is important for structural materials [1–4]. By providing an independent slip system, $\left\{10\bar{1}2\right\} < 10\bar{1}\bar{1} >$ twin acts as an important deformation mode of the hexagonal lattice [5–9], the manipulation of which has practical significance to the plasticity of hexagonal metals and alloys [10]. For instance, with the profusion and paucity of $\left[10\bar{1}2\right]$ twins in Mg and Ti, respectively, either strength or plasticity can be improved by its hindrance or promotion [11,12].

At variance with traditional models, recent studies have identified the formation of $\left[10\bar{1}2\right]$ twin via direct lattice reorientation in hexagonal Mg and Ti [13–21]. Liu et al. [13] recently reported a vertical orientation relationship between the parent and twin lattices, and proposed that the transformations at the basal/prismatic interfaces may have implications for alloy design. Ostapovets et al. [14] employed molecular statics to analyze the basal/prismatic twinning, and proposed the glide of twinning disconnections. Kumar et al. [15] reported the effect of solute elements on the structural character of the basal/prismatic interfaces in six hexagonal metals. Wu et al. [16] used *in situ* synchrotron X-ray microbeam diffraction and captured the twinning-like lattice reorientation within an individual grain inside a bulk material during strain reversal on the sub-micrometer level.

For traditional $\left[10\bar{1}2\right]$ twinning, Ishii et al. [17] divided twin nucleation into two parts, i.e., shuffle and shear, and concluded that the nucleation of $\left\{10\bar{1}2\right\} < 10\bar{1}\bar{1} >$ deformation twinning in Mg is shuffle-controlled, which requires a relatively small activation volume with more sensitive dependency on temperature and strain rate. But unlike traditional twinning, the new lattice reorientation-assisted twinning has different shear and shuffle processes, and their contribution is not yet clarified. As indicated in previous investigations [18], homogeneous nucleation of such reorientation in hexagonal Ti requires relatively large stress and strain, which hinders its popularity during deformation. A detailed investigation of its nucleation process is thus necessary. In the present work, high-throughput *ab initio* calculations are performed to systematically examine the energy paths of $\left[10\bar{1}2\right]$ twin-related lattice reorientation. By decoupling the shear and shuffle components, the characteristic of such twinning process in hexagonal metals is elucidated.

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Table 1
Cutoff energies (E_{cut}) and k-point meshes used in the calculations, the calculated and experimental lattice constants (a and c) and c/a ratios of 19 hexagonal metals and reorientation energies per atom (E). Experimental lattice constants are taken from Ref. [29].

Symbol	E_{cuf} (eV)	*k*-points	*a* (nm)		*c* (nm)		*c*/*a*		*E* (meV)
			Cal.	Exp.	Cal.	Exp.	Cal.	Exp.	
Be	450	23 × 23 × 23	0.2286	0.2266	0.3584	0.3567	1.568	1.574	51.51
Mg	350	19 × 19 × 19	0.3209	0.3194	0.5211	0.5183	1.624	1.623	16.55
Sc	550	11 × 11 × 11	0.3309	0.3320	0.5268	0.5162	1.592	1.555	48.47
Ti	450	13 × 13 × 13	0.2950	0.2936	0.4684	0.4650	1.587	1.584	38.42
Co	450	19 × 19 × 19	0.2507	0.2492	0.4069	0.4024	1.623	1.615	44.92
Y	400	15 × 15 × 15	0.3648	0.3657	0.5732	0.5675	1.571	1.552	43.71
Zr	450	11 × 11 × 11	0.3232	0.3235	0.5148	0.5168	1.593	1.597	36.09
Tc	550	15 × 15 × 15	0.2738	0.2750	0.4394	0.4399	1.605	1.599	37.77
Ru	400	13 × 13 × 13	0.2705	0.2716	0.4281	0.4279	1.583	1.576	163.96
Gd	450	15 × 15 × 15	0.3634	0.3642	0.5781	0.5737	1.591	1.575	23.01
Tb	450	15 × 15 × 15	0.3606	0.3631	0.5697	0.5680	1.580	1.564	28.54
Dy	450	15 × 15 × 15	0.3592	0.3619	0.5650	0.5633	1.573	1.556	34.93
Ho	450	15 × 15 × 15	0.3578	0.3605	0.5618	0.5593	1.570	1.552	41.54
Er	450	15 × 15 × 15	0.3559	0.3586	0.5585	0.5559	1.569	1.550	47.54
Tm	400	15 × 15 × 15	0.3538	0.3562	0.5554	0.5525	1.570	1.551	52.73
Lu	450	13 × 13 × 13	0.3505	0.3524	0.5549	0.5480	1.583	1.555	57.35
Hf	550	13 × 13 × 13	0.3195	0.3203	0.5051	0.5063	1.581	1.581	63.07
Re	600	17 × 17 × 17	0.2761	0.2775	0.4458	0.4482	1.615	1.615	79.20
Os	600	13 × 13 × 13	0.2735	0.2759	0.4391	0.4354	1.606	1.578	248.98

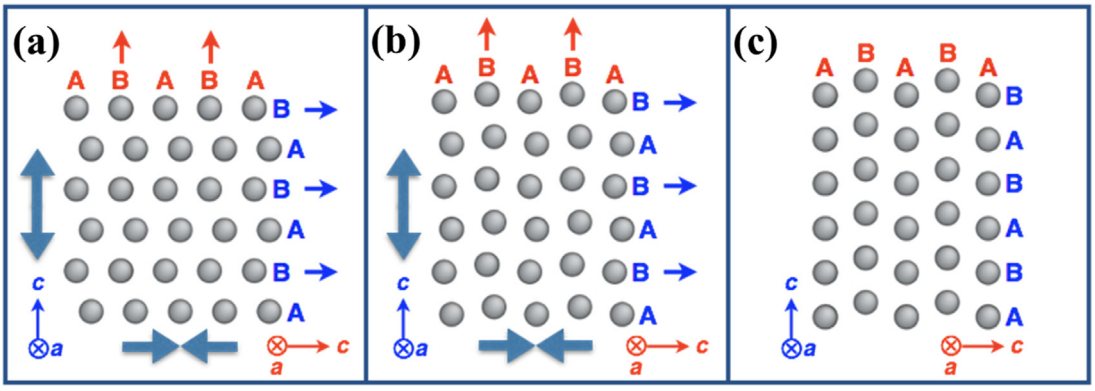

Fig. 1. Initial (a), saddle point (b), final (c) atomic configurations during the twin-related lattice reorientation. Lattices orientations are indicated. The reorientation process consists of expansion and contraction (double headed arrows), which is equivalent to pure shear, as well as individual atomic shuffles (blue and red arrows). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

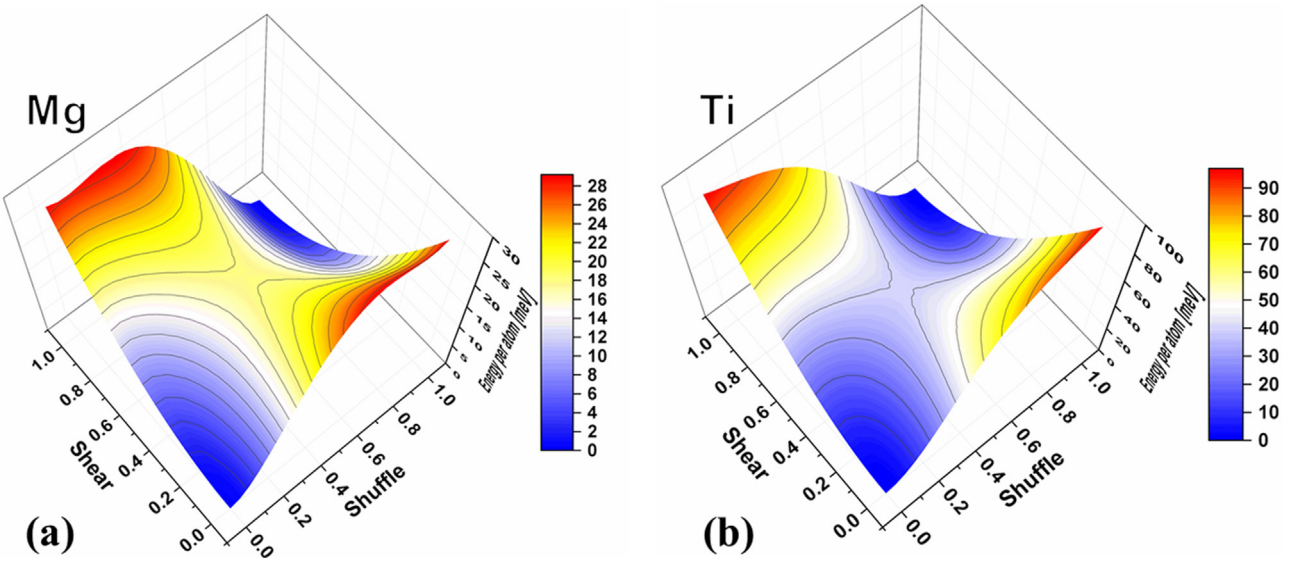

Fig. 2. Reorientation energy maps against relative shear and shuffle in Mg (a) and Ti (b).

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