Comment on "Development of an interatomic potential for the simulation of defects, plasticity, and phase transformations in titanium" J. Chem. Phys. 145, 154102 (2016)

Adam J. Ready and A. P. Sutton*
Department of Physics, Imperial College London, Exhibition Road, London, SW7 2AZ, United Kingdom

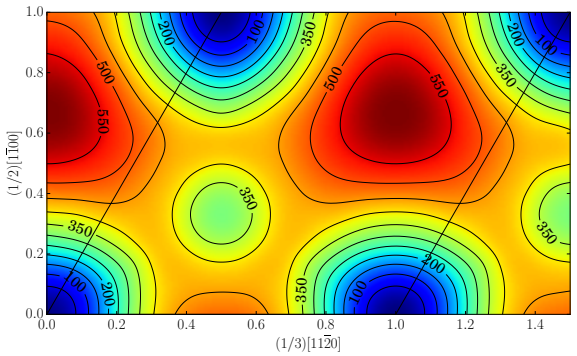
P. D. Haynes
Department of Materials, Imperial College London, Exhibition Road, London, SW7 2AZ, United Kingdom

Recently Mendelev, Underwood, and Ackland[1] (MUA) published three interatomic potentials (IPs) Ti1, Ti2, and Ti3 for pure Ti. These IPs were developed to model atomistically defects, plasticity, and phase changes in Ti. In this comment we compare quantitatively the γ-surfaces predicted by these IPs on the basal and $\{1\bar{1}01\}$ first order pyramidal or pyramidal I planes of hexagonal close-packed Ti with those we computed recently by density functional theory (DFT)[2]. We also compare with the γ-surfaces computed with the IP developed by Ackland[3], which we call Ti0. Local minima in the γ-surface[4] correspond to stable stacking faults, which indicate the possibility, depending on the energy of the local minimum, of dissociation of lattice dislocations into partial dislocations separated by the stacking fault. In addition, the slope of the γ-surface determines the force per unit area tending to constrict the core of dislocations in the slip plane[5]. The accuracy of a γ-surface is therefore of some importance for modelling plasticity on that slip plane.

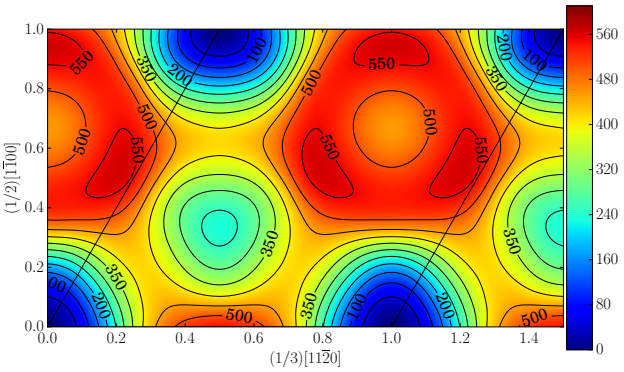
For a given translation vector $\mathbf{t}$ relaxation only normal to the fault plane was allowed. To quantify the difference between the γ-surfaces on a given plane computed by DFT, $\gamma_{DFT}(\mathbf{t})$, and by an IP, $\gamma_{IP}(\mathbf{t})$ we compute the RMS difference, as described in the Supplementary Material. The RMS differences are given in table II for each IP. For each fault the Ti0 potential is the least accurate, as expected. Of the three new IPs the Ti2 agrees best with the DFT basal γ-surface, but the Ti1 pyramidal I γ-surface agrees best with the DFT pyramidal I γ-surface.

A significant difference between the γ-surfaces on the basal plane computed with the Ti-$\{1,2,3\}$ IPs and DFT is the local maximum in the DFT surface at [1.0,0.66], which is a local minimum in the Ti-$\{1,2,3\}$ surfaces (see Fig. 1). It is also apparent that the DFT surface is more rounded than the IP-surfaces. All basal and pyramidal γ-surfaces are displayed in the Supplementary Material.

Fig. 2 shows the γ-surfaces on the pyramidal I plane computed with DFT and the Ti2 IP. The positions and energies of the I_1 fault are slightly different, as seen in Table I. There is a shallow minimum in the Ti2 γ-surface at [0.50, 0.25] with an energy of 494 mJ/m^2. In the DFT γ-surface there is a saddle point at [0.50,0.22] with an energy of 775 mJ/m^2, which becomes a shallow minimum with an energy of 681 mJ/m^2 after relaxation of all atoms



(a) Basal - DFT

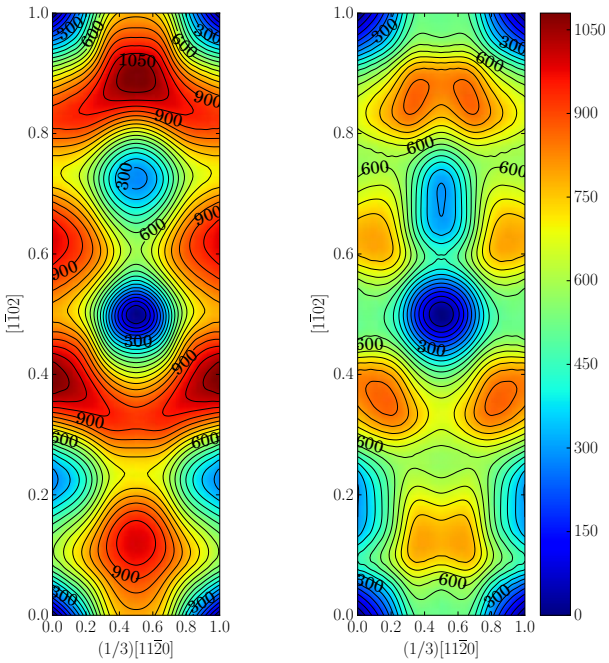


(b) Basal - Ti2

Figure 1. (Color online) Basal γ-surfaces of α-Ti computed with (a) DFT (b) Ti2 IP. (a) Reproduced with permission from Philos. Mag. **97**, 14 (2017) [2]. Copyright 2017 Informa UK Limited, trading as Taylor & Francis Group. Available at www.tandfonline.com.

parallel as well as normal to the fault. The local maximum in the DFT γ-surface at [0,0.4] is split into two local maxima in the Ti2 γ-surface. But overall the agreement between the two γ-surfaces, in terms of the locations and energies of the maxima and minima, is quite remarkable considering none of it was included in the fitting of the potentials.

If a dislocation with a line and Burgers vector lying in



(a) Pyramidal I - DFT (b) Pyramidal I - Ti2

Figure 2. (Color online) Pyramidal I γ-surfaces of α-Ti generated using (a) DFT and (b) Ti2 IP. (a) Reproduced with permission from Philos. Mag. **97**, 14 (2017) [2]. Copyright 2017 Informa UK Limited, trading as Taylor & Francis Group. Available at www.tandfonline.com.

Fault	Ti0	Ti1	Ti2	Ti3	DFT
Basal I_2	64	255	234	235	306
	[0.5,0.33]	[0.5,0.33]	[0.5,0.33]	[0.5,0.33]	[0.5,0.33]
Pyr. I_1	225	197	218	191	163
	[0,0.15]	[0,0.15]	[0,0.17]	[0,0.17]	[0,0.22]

Table I. Energies and positions of local minima in the basal and pyramidal I γ-surfaces computed using the Ti$\{0,1,2,3\}$ IPs and DFT. All energies in mJ/m^2. The positions are expressed as fractions of the lattice vectors along the x- and y-axes of the γ-surfaces shown in Figs. 1 and 2.

a particular slip plane spreads its core in the slip plane the variation in the slope of the γ-surface for the slip plane determines the structure of the dislocation core[5]. To investigate the ability of these IPs to model the core structures of such dislocations in the basal and pyramidal I planes we computed the RMS differences in the gradients of the γ-surfaces obtained with DFT and the 4 IPs. The gradients were computed using discrete Fourier transforms of the γ-surface; full details are given in the Supplementary Material.

The RMS differences are shown in table III. To gauge the significance of these differences we express them as percentages of the average slope of the corresponding DFT γ-surface.

RMS differences (mJ/m^2)	Ti0	Ti1	Ti2	Ti3
Basal	107	87	57	62
Pyramidal I	236	116	172	190

Table II. RMS differences between γ-surfaces on basal and pyramidal I planes computed with DFT and Ti-$\{0,1,2,3\}$ IPs.

RMS differences (%)	Ti0	Ti1	Ti2	Ti3
Basal	100.0	73.8	73.2	85.7
Pyramidal I	60.9	52.5	56.9	77.6

Table III. RMS differences between gradients of the γ-surfaces computed with DFT and Ti-$\{0,1,2,3\}$ IPs, expressed as a percentage of the average slope of the corresponding DFT γ-surface.

In conclusion, the new IPs Ti-$\{1,2,3\}$ do provide better agreement than the Ti0 IP, with γ-surfaces on the basal and pyramidal I planes computed with DFT. However, both the energies and the slopes of γ-surfaces computed with *all* the potentials show large deviations from those computed with DFT. It remains to be seen whether these deviations are so great they severely limit the accuracy of the modelling of slip on basal and pyramidal I planes. Finally, we note that although Mendelev *et al.* found it impossible to *fit* both low and high temperature properties of Ti with a single potential, recent DFT calculations by Zhang *et al.*[6] have *predicted* both in good agreement with experiment.

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* a.sutton@ic.ac.uk

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