Erratum: Molecular dynamics study of the threshold displacement energy in vanadium [Phys. Rev. B 67, 134114 (2003)]

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Following manuscript publication, P. Vajda has brought to our attention the existence of experimental references on the threshold displacement energy in vanadium,[29,31–35] which were inadvertently missed in our literature review. Additionally, P. Vajda also brought to our attention our erroneous description of literature data as being experimentally obtained, when in fact they were produced by computer simulation. Thus, we present:

(i) a modified version of Fig. 2 that includes the measured TDE values in vanadium along the low index ⟨100⟩, ⟨110⟩, and ⟨111⟩ directions due to Kenik and Mitchell;[29]

(ii) a modified caption and legend for Fig. 2 that clarifies our erroneous description of literature data [Fe was listed as Exp. (experimental) rather than Sim. (simulation)];

(iii) eight additional references (listed below as Refs. 28–35); and

(iv) a modified and extended discussion, which should replace paragraph 2 of Sec. IV. DISCUSSION AND CONCLUSIONS of the original manuscript.

MODIFICATION TO SEC. IV. DISCUSSION AND CONCLUSIONS

Paragraph 2 should be modified to the following three paragraphs:

A comparison of the computed threshold displacement energy with experimental values for V (Ref. 29) and Mo (Ref. 23), and computer simulation results for bcc Fe (Ref. 28) is shown in Fig. 2 for the low index directions. MD simulations for Fe and Mo generally reproduce the experimental data.[12,13,26,28] The ordering of low index directions, e.g., lowest energy in ⟨100⟩ followed by ⟨111⟩ and then ⟨110⟩, obtained in these simulations agrees well with the experimental results for vanadium.[29] However, the absolute displacement energies differ substantially, and are much higher in the experiment. This discrepancy likely results from many factors, including the comparison between short timescale MD simulations, which measure the minimum displacement energy to produce closely separated Frenkel pairs, with experimental measurements of displacement energy associated with the formation and growth of visible defect clusters in the transmission electron microscope at room temperature. Notably, the magnitude of the TDE obtained in our simulations does agree well with previous simulations reported by DiCarlo,[30] although in that case the relative ordering of ⟨100⟩ to ⟨111⟩ directions was reversed. It is possible that the directional reversal between these two simulation studies is related to the use of an improved many-body interatomic potential in this work.

Miller and Chaplin[31] and Jung and Lucki[32] have reported effective minimum TDE values of 26±2 and 25 eV for vanadium, respectively. These experimental measurements were obtained at temperatures below 20 K, compared to room temperature for the directional dependent results presented in Fig. 2. The minimum TDE values[31,32] are less than the directional TDE values measured by Kenik and Mitchell,[29] but are still larger than those obtained from MD. In the MD simulations, defect production and the TDE was determined in a series of simulations of ten picosecond duration, which limits the occurrence of many closely correlated recombination processes, except for the recombination of colinear Frenkel pairs in the ⟨111⟩ direction by rapid one-dimensional crowdion motion. Thus, it is possible that the lower TDE values and the temperature independence obtained in this study are the result of the short MD time scales. As well, Coltman *et al.*[33] report that "3.8 K is probably not cold enough to stabilize all damage in V,"[33] and therefore, it is likely that the close-pair recombination that occurs during irradiation of V can further explain some of the discrepancy.

Experimental observations of low-temperature interstitial mobility at 3.8 K,[33] and the large vacancy–self-interstitial recombination volume of 690 to 810 atomic volumes reported by Vajda and Biget[34] are not entirely consistent with the temperature independence of the TDE or the observed Frenkel pair stability at high T observed in the MD simulations, unless these relate directly to the short simulation

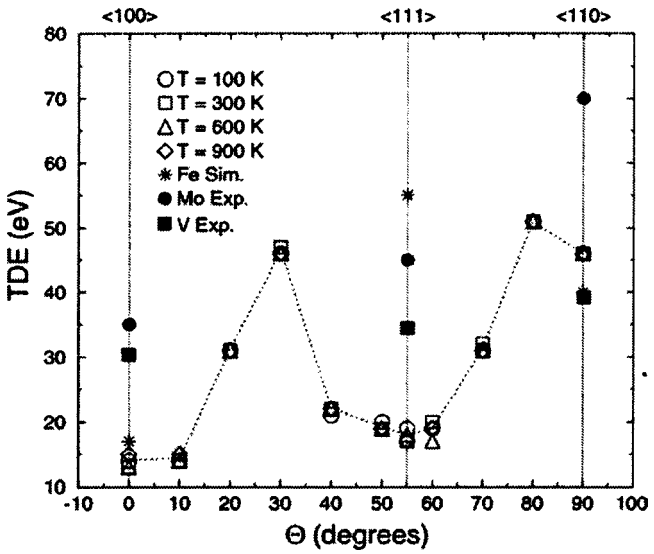

FIG. 2. Variation of the threshold displacement energy (TDE) with recoil orientation and temperature from MD simulations (open symbols). Simulation results for Fe (Ref. 28) and experimental results for V (Ref. 29) and Mo (Ref. 23) are shown for comparison. The dashed line is a guide connecting the average of the MD results.

times. While it is possible that the observed temperature independence, as well as the high-temperature defect stability, is a direct result of the short time scale MD simulations, which necessarily exclude recombination processes involving either vacancy migration or self-interstitial rotation as mentioned in the original manuscript, this area requires additional study. Thus, we conclude that the results obtained in this work on the directional ordering of the TDE are consistent with the available experimental data for vanadium and to a lesser extent with the absolute values, although the temperature independence of the TDE and the Frenkel pair stability at high temperatures observed in this work requires further study.

The comparison of these MD simulation results of the TDE in V to MD simulations of other bcc metals[12,13,26,28] shows that the directional anisotropy is comparable in Mo but the TDE ordering in ⟨110⟩ and ⟨111⟩ orientations is different in Fe. The reversal of ⟨110⟩ and ⟨111⟩ ordering is somewhat puzzling, since all three metals exhibit easy one-dimensional motion in the ⟨111⟩ crowdion direction, even though the stable self-interstitial is a ⟨110⟩ dumbbell in both Mo and Fe. Possible explanations for the disparity of these three metals may involve the self-interstitial properties, or possibly anisotropy of the elastic constants, but this also requires further investigation.

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