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Erratum: Evaluation of first-principles techniques for obtaining materials parameters of α-uranium and the (001) α-uranium surface [Phys. Rev. B 77, 094119 (2008)]

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In my paper I stated that the surface energy of α-U(001) was 1.4 $\mathrm{J/m^2}$ as determined by density functional theory. This value and the values tabulated for various levels of slab calculation were incorrectly calculated, although the formula for the surface energy given in the previous publication is correct.

$$\gamma = (E_{slab} - NE_{bulk})/2A$$

γ is the surface energy, E_{slab} is the energy of the entire slab, N is the number of atoms in the slab calculation, E_{bulk} is the energy of the bulk crystal per atom, and A is the surface area of the slab.

The correct values are tabulated below, and should replace the surface energies given in Table V of the previous work. The remaining values in Table V of the previous work are correct as given (Table I).

Some aspects of the discussion following the presentation of surface energies also need to be revised from the previous publication. These aspects are revised in the following.

Estimates of the surface-energy of polycrystalline uranium range between 1.000 and 1.490 J/m based on theoretical correlations between physical parameters such as the heat of sublimation and atomic volume.[1,2] An investigation of fission bubbles in α-uranium yielded an approximate surface energy of 1.0 ± 0.5 J/m.[3,4] The surface energy arising from the PAW calculations described in my paper and recalculated herein of 1.8 $\mathrm{J/m^2}$ is higher than these estimates. Further investigation is therefore required to verify the α-U(001) surface energy.

By utilizing the model of Hayes and Carter, it is possible to relate the (001) surface energy ($\gamma = 1.8\ \mathrm{J/m^2}$), the bulk-interlayer distance (d=2.447 Å) and the c_{33} elastic constant (c_{33}=331 GPa, this work), to the cohesive properties of the (001) planes.[5] Succinctly, this model imposes the crack formation criterion that the elastic strain energy imposed upon an elongated crystal must exceed the surface energy of the crystal. Thus, at some elongation, surface formation via crack development must become more favorable than continuously straining the crystal. Two parameters arise from this model: the critical elongation, and the stress required to achieve that elongation (critical peak traction). Although α-uranium is a metal, and will fail via plastic deformation (movement of dislocations) the brittle fracture value provides a guide to the 'yield stress' of the material, at which point the elastic limit is reached and plastic modes will take over. The important modes of failure via plastic deformation modes and/or intergranular cracking could be modeled at a later stage using interatomic pair-potential techniques. The simple elastic model presented by Hayes and Carter determines the critical crack opening displacement by equalizing the elastic energy density imposed by a critical strain value to the surface energy yielded upon complete fracture.[5] The procedure is analogous to the Griffith equation for crack propagation.[6] The resulting critical opening displacement is $\bar{\delta}_r = 2\sqrt{\gamma w / c_{33}}$, where w is the sample width. As such the critical crack opening is dependent on the sample-width, as the elastic strain energy is a volume property, compared to the surface energy, which is a two-dimensional surface quantity. For a 10 μm single-crystal, therefore, in the absence of dislocations, brittle-failure would occur at a critical displacement of 147 Å. The related critical peak traction is $\bar{\sigma}_r = c_{33}\bar{\delta}_r / w$, or 487 MPa for a 10 μm single-crystal. The computed value is closer to the value determined by Hayes and Carter for the α-Al_2O_3 single crystal than that for Al(111), consistent with the semi-plasticity (rather than total-plasticity) of α-uranium as it indicates that the metal is more similar to the aluminum oxide than the aluminum metal.[5,7] Ref. 7 cites a reported yield stress of 345 MPa for polycrystalline α-uranium, which is 21% lower than the 437 MPa obtained

TABLE I. Surface energy, γ ($\mathrm{J/m^2}$) for model N-layer α-uranium (001) oriented slabs.

N	γ
3	1.824
4	1.824
5	1.808
6	1.776
7	1.808

using the measured, room temperature c_{33} and the above equation. This reduction can be attributed to the contribution of plastic failure modes.

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