Erratum: Determination of activation parameters for dislocation formation from a surface in fcc metals by atomistic simulations [Phys. Rev. B 78, 064109 (2008)]

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We found an error in the proposed elastic model which describes the energy of an elliptic half-loop dislocation nucleated from a surface step as a function of its size and of the applied strain. In fact, in the expression (4), there should be no $(1-\nu)$ factor at the denominator. The correct expression is therefore

$$E_\epsilon = -\mu b(1+\nu)e\pi R^2 \cos\theta_1 \cos\theta_2 \epsilon \tag{4}$$

As a consequence, the correct Eq. (6) is now

$$R_c = \frac{1}{16\pi e(1+\nu)\cos\theta_1 \cos\theta_2 \epsilon} \times \left\{ \frac{b(2-\nu)}{(1-\nu)} \left[\ln\left(\frac{8m\alpha R_c}{b} \right) - 1 \right] + \frac{8e}{\mu b} \left(\pi R_c - \frac{4}{3}\sigma_s \right) \right\} \tag{6}$$

This error only concerns the elastic model, and the critical radius values obtained from atomistic simulations (reported in the original Fig. 3) remain valid. However, the corrected elastic model has to be refitted on these data. Assuming that $\alpha=2$, we now found that the best agreement is obtained for $m=0.5$ and an ellipticity factor $e=1.05$. These new parameters are very close to the previous ones. The corresponding curve is shown on the corrected Fig. 3.

In addition, the activation volume variation as shown in the Fig. 7 of the original paper must be updated too, since it is derived from the variation of the activation energy as given by the elastic model. The correct activation volume curve is shown in the Fig. 7 presented here. Note that the correct variation has the same shape than the previous one, but the range of data is now different. As a consequence, in the text of the original manuscript, it was written that the athermal threshold was obtained

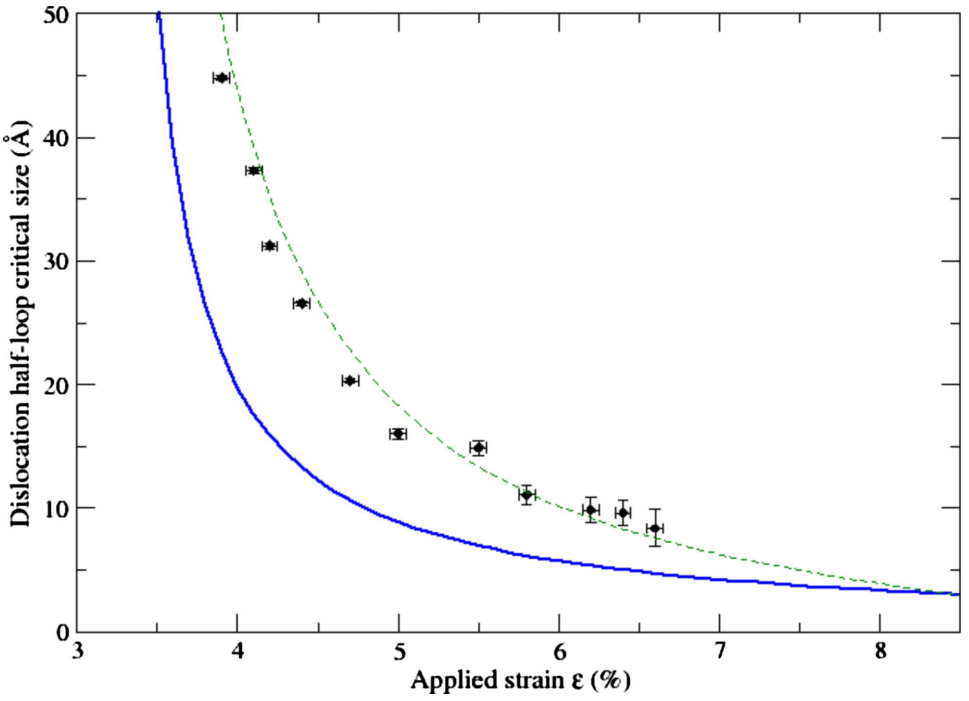

FIG. 3. (Color online) Critical radius R_c vs elongation obtained by MD (diamonds). The full line is the critical distance obtained from elasticity theory for a straight dislocation [Eq. (2)]; the dashed line is the one obtained from our fitted elastic model for an elliptic dislocation [Eq. (6)].

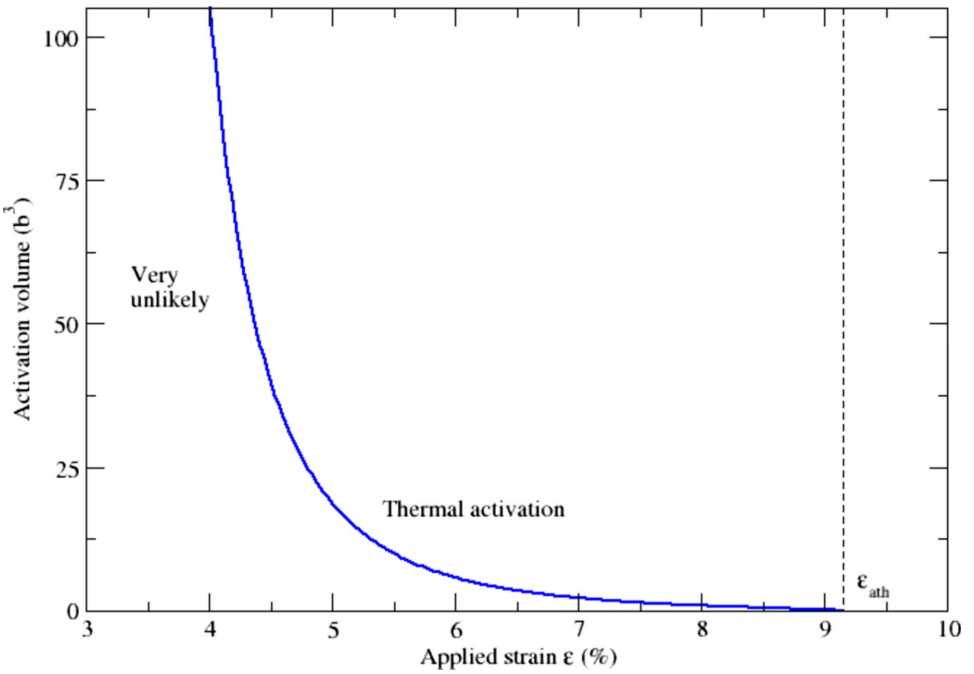

FIG. 7. (Color online) Activation volume as a function of the applied strain, calculated using the proposed elastic model.

for ϵ=9.3%. The correct value is now ϵ=9.15%. Also, it was proposed that between 3.2% and 9.3%, the nucleation process was thermally activated. According to the updated results, it should be understood that the nucleation process is thermally activated between approximately 5% and the athermal threshold, 9.15%.

Finally, we point that although this mistake leads to modifications of numerical values, it did not undermine any of the conclusions put forward.

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