MULTISCALE MODEL. SIMUL.
Vol. 7, No. 2, pp. 1003–1003

ERRATUM: PREDICTION OF DISLOCATION NUCLEATION DURING NANOINDENTATION BY THE ORBITAL-FREE DENSITY FUNCTIONAL THEORY LOCAL QUASI-CONTINUUM METHOD*

ROBIN L. HAYES†, MATTHEW FAGO‡, MICHAEL ORTIZ‡, AND EMILY A. CARTER§

Abstract. In this erratum, we correct typographical errors in the equation for the ion-electron stress in [Hayes et al., *Multiscale Model. Simul.*, 4 (2005), pp. 359–389].

DOI. 10.1137/080727531

In [1], (A.3) should have been written

$$\sigma^{\mathrm{Ext}}_{\alpha\beta} = -\frac{1}{\Omega}\sum_{g\neq 0}\sum_{I}\rho(\vec{g})\frac{g_\alpha g_\beta}{|\vec{g}|}\frac{\partial V^{loc}_{Ie,I}(g)}{\partial g}\exp(i\vec{g}\cdot\vec{R}_I) - \delta_{\alpha\beta}\frac{E_{\mathrm{Ext}}}{\Omega}.$$

The above (correct) equation, previously derived by Nielsen and Martin [2], was used during all of the simulations reported in this work.

REFERENCES

[1] R. L. HAYES, M. FAGO, M. ORTIZ, AND E. A. CARTER, *Prediction of dislocation nucleation during nanoindentation by the orbital-free density functional theory local quasi-continuum method*, Multiscale Model. Simul., 4 (2005), pp. 359–389.

[2] O. H. NIELSEN AND R. M. MARTIN, *Stresses in semiconductors: Ab initio calculations on Si, Ge, and GaAs*, Phys. Rev. B, 32 (1985), pp. 3792–3805.

*Received by the editors June 16, 2008; accepted for publication June 23, 2008; published electronically October 17, 2008.

http://www.siam.org/journals/mms/7-2/72753.html

†Department of Chemistry, New York University, New York, NY 10003 (robin.hayes@nyu.edu).

‡Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, CA 91125 (fago@caltech.edu, ortiz@aero.caltech.edu).

§Department of Mechanical and Aerospace Engineering and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544-5263 (eac@princeton.edu).