ERRATUM

Erratum to: Molecular dynamics simulation of thermal accommodation coefficients for laser-induced incandescence sizing of nickel particles

K. J. Daun · J. T. Titantah · M. Karttunen

Published online: 14 August 2013
© Springer-Verlag Berlin Heidelberg 2013

Erratum to: Appl Phys B (2012) 107:221–228
DOI 10.1007/s00340-012-4896-x

In the continuation of our research [1], we discovered an error in the implementation of the Quantum Sutton-Chen (Q-SC) [2–5] potential used to define the nickel surface. This error overestimated the many-body attractive force between the nickel atoms, causing the nickel to remain in solid phase when it should have been liquid. When coupled with the ab initio-derived Morse pairwise potential between the argon and nickel atoms, the corrected Q-SC model produces a larger thermal accommodation coefficient compared to the value in ref. [1]. The corrected values are summarized in the table below (Table 1).

Figure 1 shows the probability that a gas molecule hits the surface a specified number of times during a scattering event. The ab initio-derived Morse potential predicts that the gas molecule will scatter almost directly, while the erroneously deep LJ 6–12 potential predicted by the Lorentz Berthelot rules results in a more prolonged interaction.

The online version of the original article can be found under doi:10.1007/s00340-012-4896-x.

K. J. Daun (✉)
Department of Mechanical and Mechatronics Engineering,
University of Waterloo, 200 University Avenue W.,
Waterloo, ON, Canada N2L 3G1
e-mail: kjdaun@uwaterloo.ca

J. T. Titantah
Department of Applied Mathematics, University of Western
Ontario, 1151 Richmond St. N., London, ON, Canada N6A 5B

M. Karttunen
Department of Chemistry, University of Waterloo,
200 University Ave. W., Waterloo, ON, Canada N2L 3G1

Table 1 Revised accommodation coefficients for Ni/Ar system

	Morse (ab initio)	Lennard–Jones 6–12 (Lorentz–Berthelot)
α_n	0.60 ± 0.07	0.99 ± 0.10
α_t	0.42 ± 0.05	0.85 ± 0.09
α	0.51 ± 0.04	0.92 ± 0.05
N_{hits}	1.8 ± 0.1	7.4 ± 0.6

Fig. 1 Probability of an argon molecule undergoing a specified number of hits before scattering from a nickel surface

Figure 2 shows that the probability densities of scattered trajectories found using kernel density estimation. The distributions for the normal and tangential scattered velocities corresponding to the ab initio-derived potential are closer together compared to the curves shown in [1], since the liquid state of the nickel droplet results in a larger α_t . Two-temperature Maxwell–Boltzmann distributions are in good agreement with the corresponding probability densities, but for clarity, the corresponding Maxwell–Boltzmann

Fig. 2 Scattered molecular speeds obtained from molecular dynamics

distributions are only shown for 1,250 and 2,500 K, representative of the partial and complete accommodation scenarios predicted by the *ab initio*- and Lorentz–Berthelot-derived potentials, respectively.

The main conclusion of the original paper that the Lorentz–Berthelot combining rules produce a gas/surface potential that overestimates the accommodation coefficient is unaffected by this error.

References

1. K.J. Daun, J.T. Titantah, M. Karttunen, *Appl. Phys. B* **107**, 221 (2012)
2. T. Çagin, Y. Kimura, Y. Qi, H. Li, H. Ikeda, W.L. Johnson, W.A. Goddard III, *MRS Symp. Ser.* **554**, 43 (1999)
3. Y. Qi, T. Çagin, Y. Kimura, W.A. Goddard III, *Phys. Rev. B* **59**, 3527 (1999)
4. A. Sutton, J. Chen, *Philos. Mag. Lett.* **61**, 139 (1990)
5. H. Rafii-Tabar, A. Sutton, *Philos. Mag. Lett.* **63**, 217 (1991)