

**Erratum: “Modeling crystal growth from solution with molecular dynamics simulations: Approaches to transition rate constants” [J. Chem. Phys.136, 034704 (2012)]**

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## Erratum: “Modeling crystal growth from solution with molecular dynamics simulations: Approaches to transition rate constants” [J. Chem. Phys. 136, 034704 (2012)]

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A minor error in the program used to determine the surface-diffusion rate constants lead to the underestimation of the surface-diffusion rate constants published in Table IV of the original article.<sup>1</sup> These quantities represent the rate constants for transitions of particles between nearest neighbor surface sites and can potentially be used in kinetic Monte Carlo simulations. A second molecular dynamics (MD) simulation has been performed at 300 K on an equilibrated system for 16 ns. The resulting trajectory has been correctly analysed and the surface-diffusion rate constants are given in Table I.

TABLE I. Equilibrium surface-diffusion rate constants, in units of  $s^{-1}$ , from a 16 ns MD simulation at 300 K and 77 MPa. The upper diagonal diffusion rates have been determined using the detailed-balance condition and the corresponding reverse reaction.

Coordination state	4	5	6	7	8
4	$2.6059 \times 10^8$	$1.7021 \times 10^8$	$3.2075 \times 10^8$	$5.9988 \times 10^7$	...
5	$7.9474 \times 10^7$	$8.4501 \times 10^7$	$2.3678 \times 10^8$	$1.8777 \times 10^8$	...
6	$7.4377 \times 10^7$	$1.3284 \times 10^8$	$1.3067 \times 10^8$	$6.6340 \times 10^7$	...
7	$8.7218 \times 10^6$	$7.8258 \times 10^7$	$4.8405 \times 10^7$	$4.4861 \times 10^7$	...
8	...	...	...	...	...

One notes the increase for almost all of the rate constants. From the programming error we expect an increase by a factor of roughly two. The average increase of all the newly reported rates is 2.26. Due to the low number of surface-diffusion events observed in the simulations, the statistical uncertainty of the rate constants is quite large. In particular, some of the smaller rate constants appear to be affected more strongly (*e.g.*,  $4 \rightarrow 4$ ,  $5 \rightarrow 7$ ,  $7 \rightarrow 5$ ). However, one should keep in mind that these surface-diffusion rate constants are orders of magnitude smaller than the governing growth and dissolution rate constants and are therefore especially affected by the mentioned statistical uncertainty.

The new values do not alter any of the conclusions or other results of the original paper and from our own tests, the original rate constants remain representative. In nearest neighbor kinetic Monte Carlo simulations reported elsewhere,<sup>2</sup> where the original rate constants were used, it has been noted that role of nearest neighbor diffusion appears to be limited to solely reducing the growth rate by spending time on transitions where no growth or dissolution occurs. At 300 K only a minor impact of surface diffusion on the growth rate and roughness was observed, which would likely be increased by having larger surface-diffusion rate constants, but again only by a small amount as the relative contribution of the surface-diffusion rate constants to the overall rate constant remains small.

We are grateful to Dr. E. Elts for bringing the programming error to our attention.

<sup>1</sup>A. M. Reilly and H. Briesen, *J. Chem. Phys.* **136**, 034704 (2012).

<sup>2</sup>A. M. Reilly and H. Briesen, *J. Cryst. Growth* **354**, 34–43 (2012).

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