Supplemental Material for "Spatially-correlated Site Occupancy in the Nonstoichiometric Meta-stable ε-$Al_{60}Sm_{11}$ Phase during Devitrification of Al-10.2 at.% Sm Glasses"

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The constrained molecular dynamics (MD) simulations

To constrain the Sm diffusion during the MD simulations, an additional potential $V(\mathbf{r}) = k|\mathbf{r} - \mathbf{r_0}|^6$ was applied on Sm atoms. As shown in Fig. S1(a), the potential profile is flat at the bottom and increase quickly when $|\Delta r|$ becomes larger. The free region of the potential well, characterized by r_c, is controlled by the parameter k. This can also be verified by computing the square root of the mean square displacement (MSD) of the constrained Sm atoms during the MD simulation, which is shown in Fig. S1(b). It can be seen that the constrained Sm displacement matches well with the flat region of the potential profile.

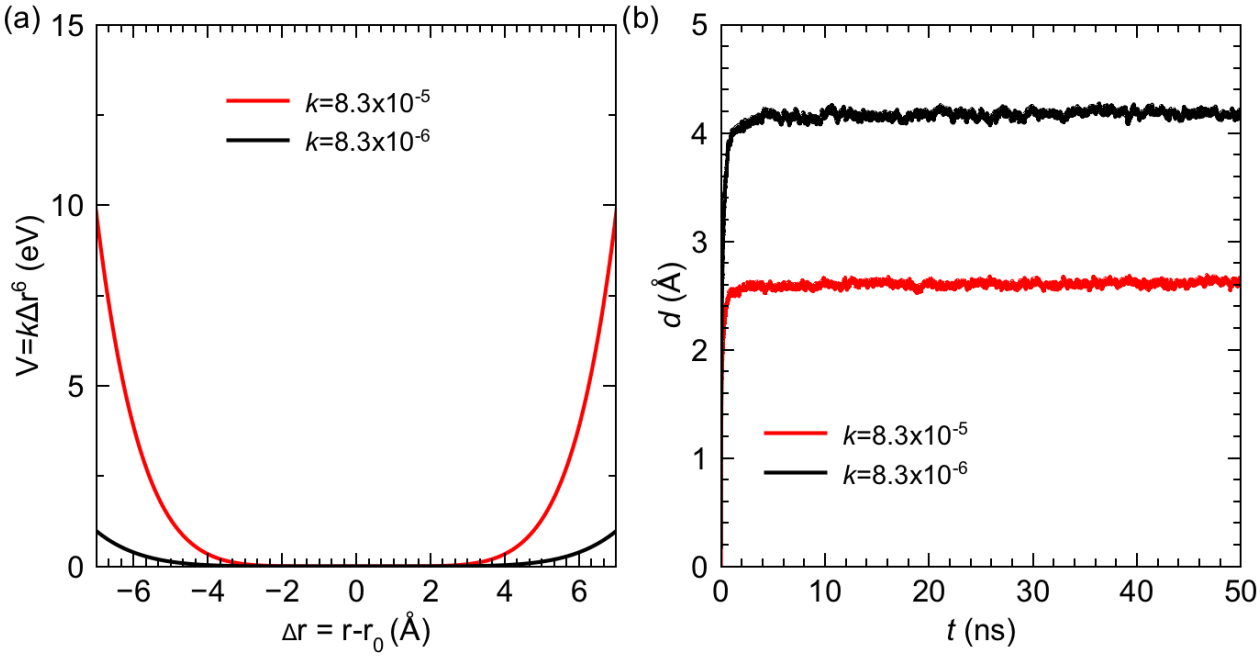

Fig. S1 (a) The profile of the potential $V(\mathbf{r}) = k|\mathbf{r} - \mathbf{r_0}|^6$. The flat region ($r_c$) changes with the parameter k. The red and black curves correspond to $r_c = 2.6$ Å and 4.2 Å, respectively. (b) The square root of the mean square displacement of the Sm atoms constrained by the potential well with different values of k.