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Modeling the relationship between melting point of the metal nanoparticle and its surface curvature

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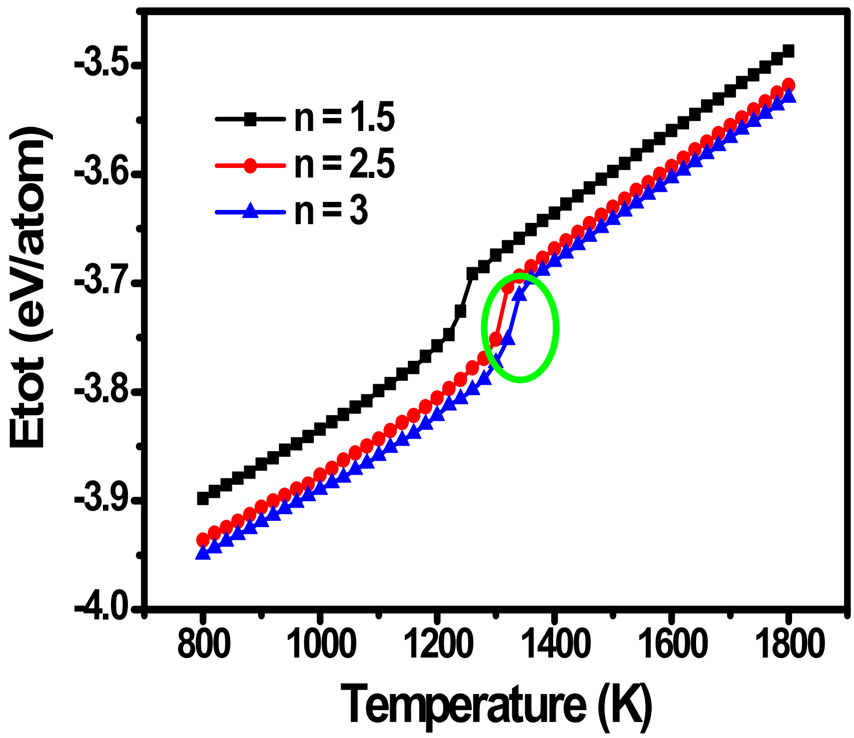

Figure S1. Total energy per atom as a function of temperature for different ratios of length to diameter. It is indicated that when the length-to-diameter ratio of the embedded particle is larger than 2.5, the melting point of the particle is independent on its length.

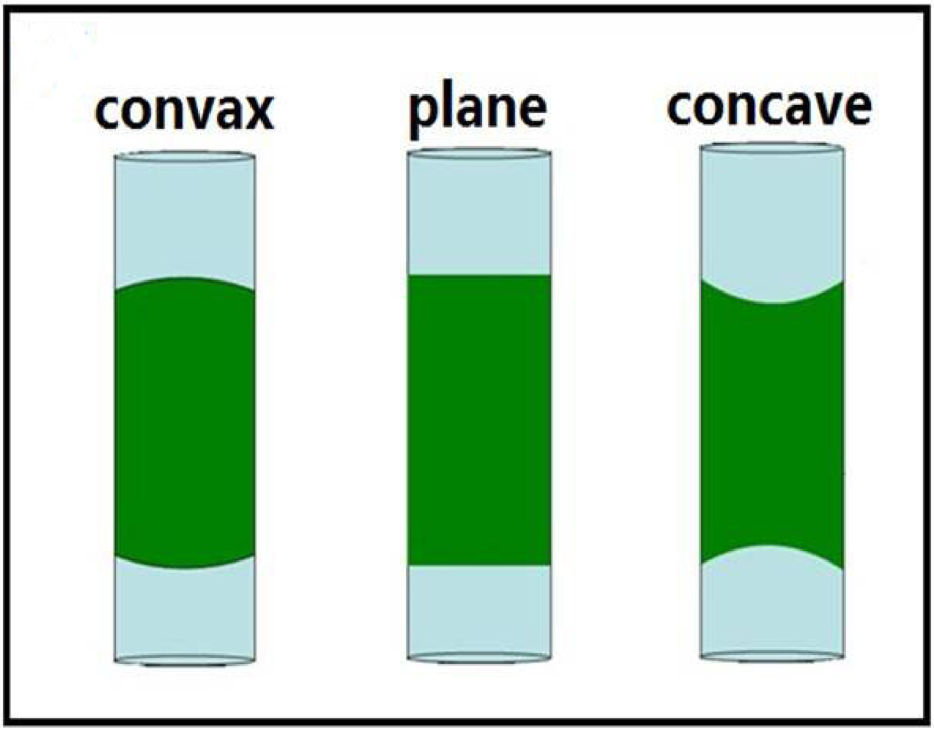

Figure S2. Schematic of the three typical surfaces. With the increase of the confinement-metal interaction by increasing the potential parameter from ε = 0.1 eV to ε=0.8 eV, the surface curvature of the Fe melt gradually decreases and the morphology represents three typical statuses (convex, plane and concave).

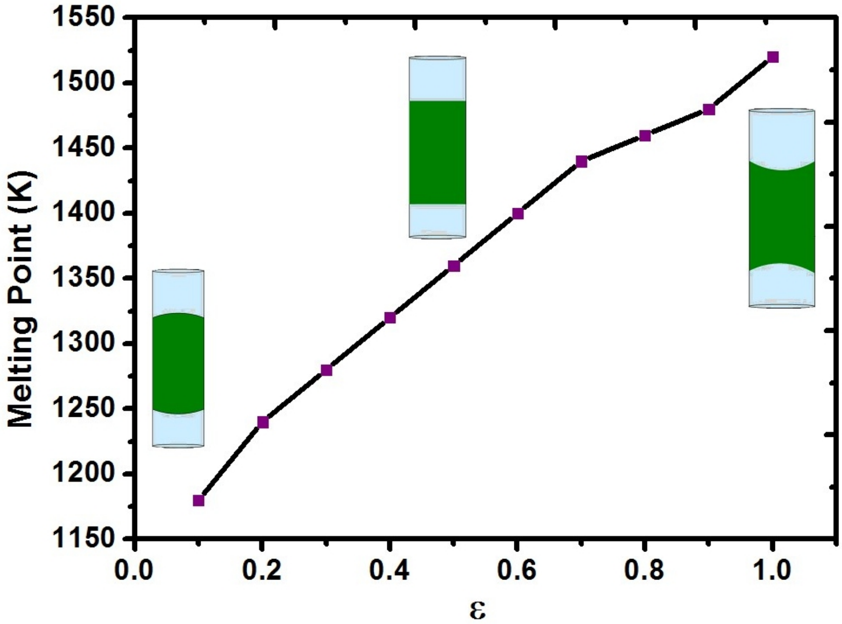

Figure S3. Variation of the melting point of Fe_{1000} in nanoconfinement with the confinement-metal interaction strength increasing from ε=0.1 to ε=1.0 eV. The diameter of the confinement is 16 Å. It can be seen that the curve represents a linear relationship between the melting point and the interaction strength ε.

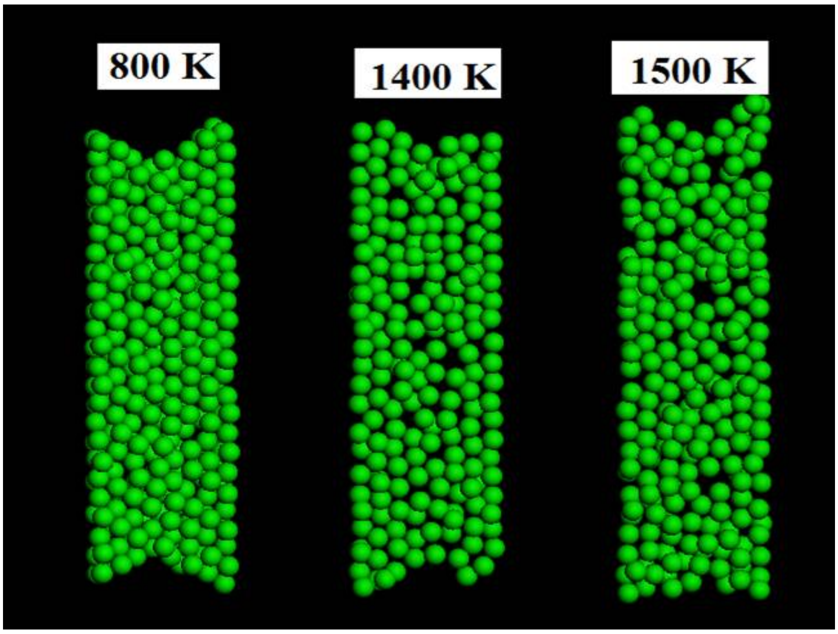

Figure S4. The evolution of the Fe_{1000} inner structure during the melting processing at ε=1.0. With the temperature rising, the embedded particle slowly melts from inner to interface and then completely melts. This is another evidence of the inner-diffusing melting.