

Supplementary Material of:

Thermal Behavior in FeCuCrCoNi High Entropy Alloys 4

Nanoparticles: An Atomistic Approach

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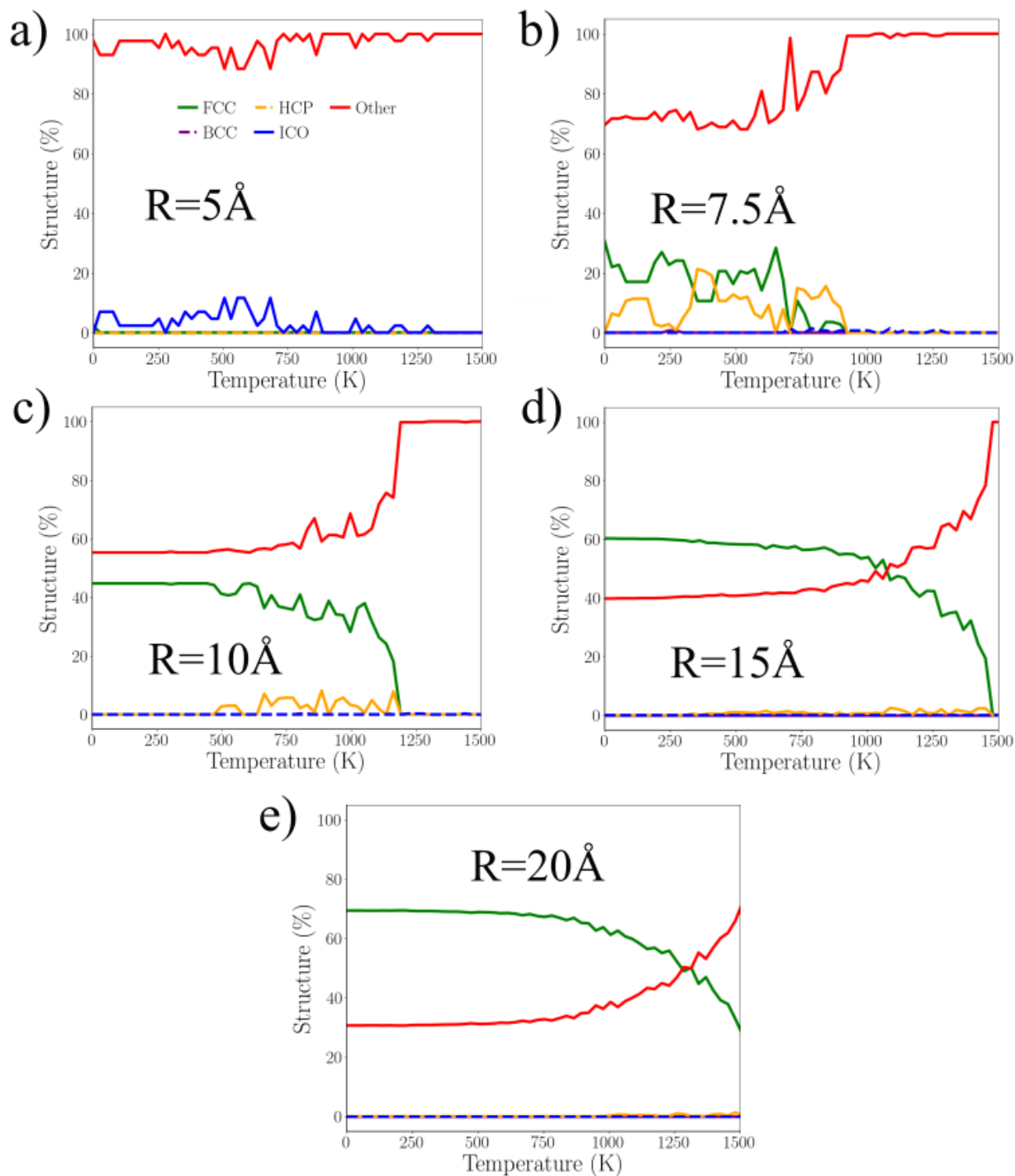


Fig S1. Crystalline structure as a function of temperature for different nanoparticle sizes. a), b), c), d) y e) correspond to radius of 5, 7.5, 10, 15 y 20 Å, respectively. Crystalline structure was identified with PTM algorithm.

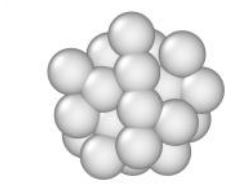
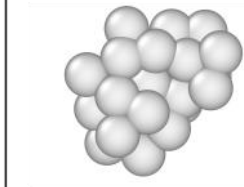
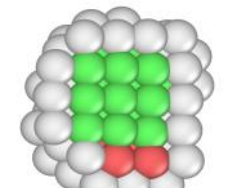
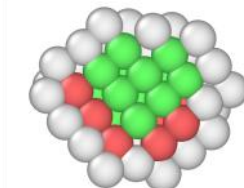
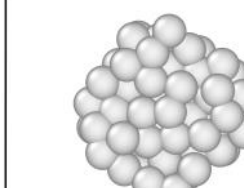
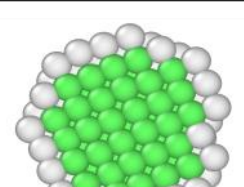
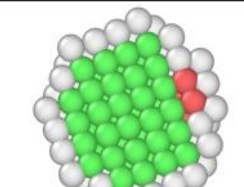
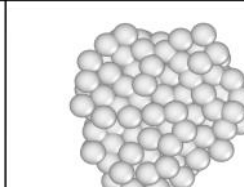
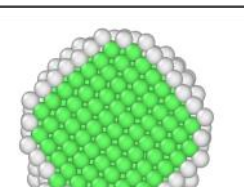
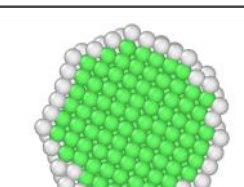
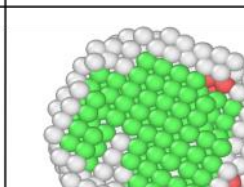
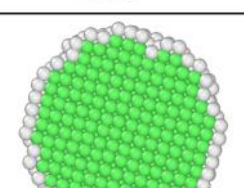
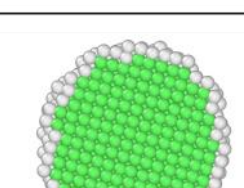
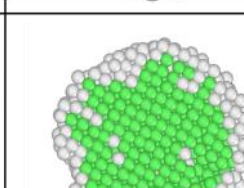
	● Other 300 K	● FCC 500 K	● HCP 1300 K
5 Å			
7.5 Å			
10 Å			
15 Å			
20 Å			

Fig. S2. Illustration of the nanoparticles as a function of temperature (K) and nanoparticle size (Å). The figure shows the nanoparticle with a cross-section along the uniaxial Y direction and the predominant crystal structure of each atom.

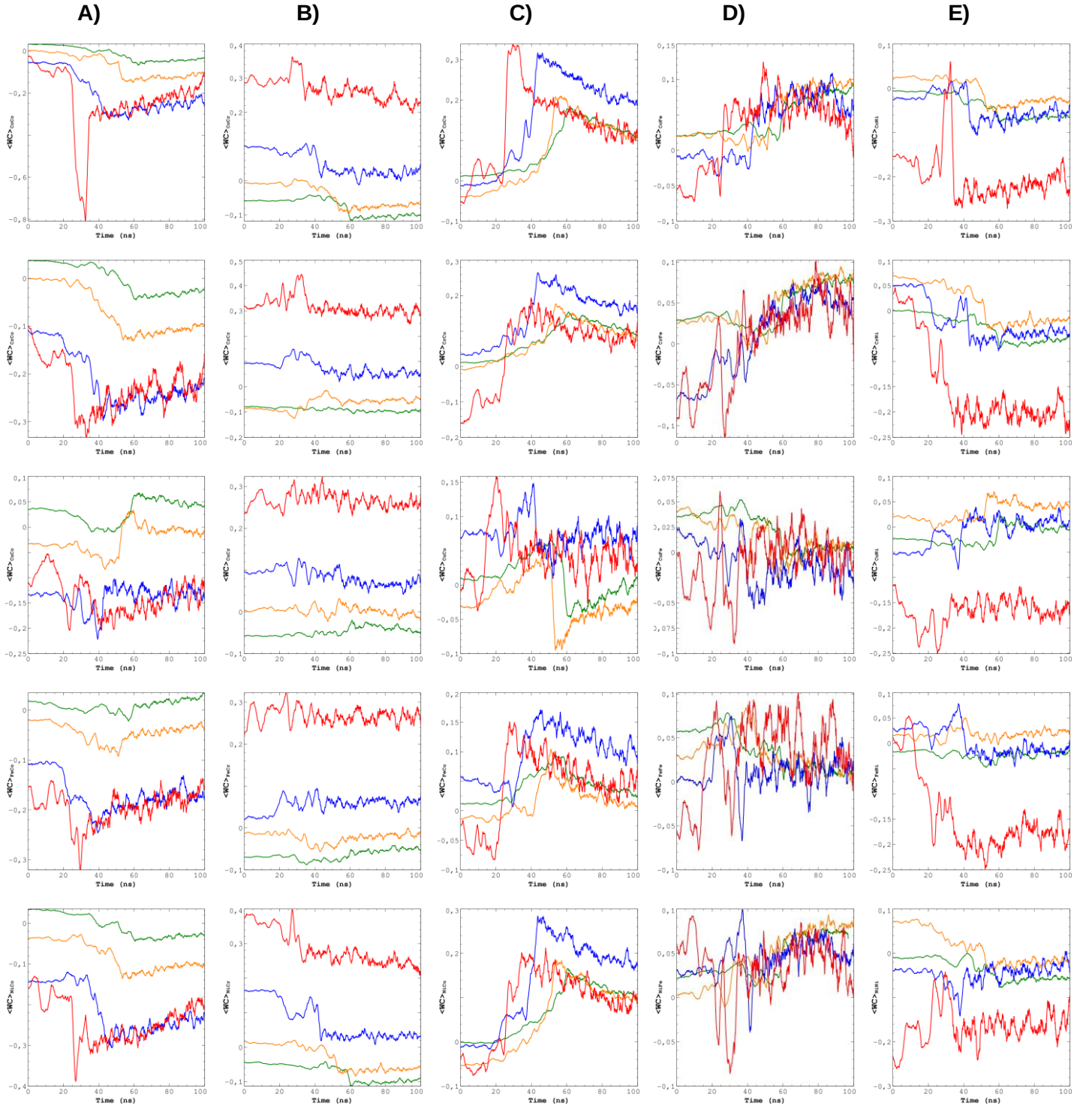


Fig S3. Curves of the WC parameter for each atom in NP as function of time and different sizes. $\langle WC \rangle_{xy}$ is the computed WC of atom y respect to atom x , where $x, y = \{Co, Cr, Cu, Fe, Ni\}$. The graphs in columns A), B), C), D), and E) correspond the WC curves computed for Cu, Cr, Cu, Fe, and Ni atoms, respectively.