Study of the threshold crystallization rate of Si-Al and Si-Au nanoparticles with molecular dynamics method

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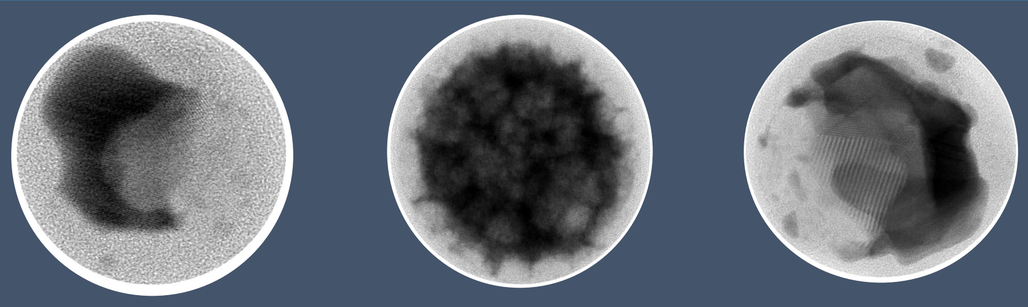
Motivation

Silicon nanoparticles make great interest for their variable in combination with metal adds. Recently the technique of laser printing was developed, which allows to create nanoparticles (NP) with properties needed. To analyze structure more precisely the molecular dynamics method was added. The potential optimized was developed only in 2020.

**S. Starikov , I. Gordeev et al.* // Comput. Mater. Sci., 184 (2020) 109891

Experimental data



These photos were obtained for Si-Au NPs in the experiments, the question is which is the situation inside Si-Al NPs.

**A.Larin, A.Nominé, et al.* // Nanoscale, 2020, 12, 1013

Simulation details

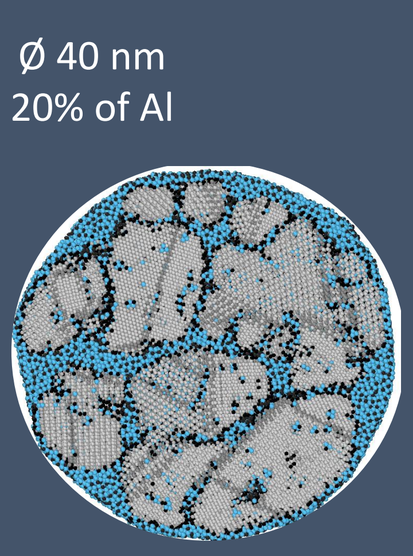
The potential presents complicated structure, the angular-dependent format.

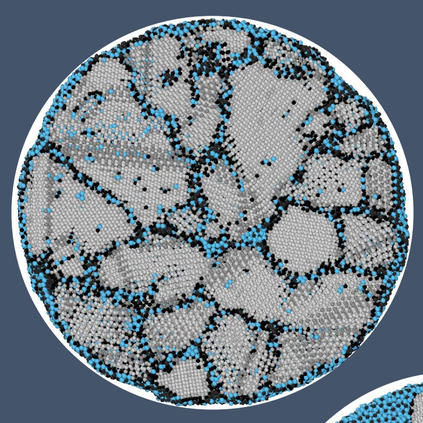
$$E_i = \frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}(r_{ij}) + F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_s(\mu_i^s)^2 + \frac{1}{2}\sum_{s,t}(\lambda_i^{st})^2 - \frac{1}{6}\nu_i^2$$

$$\mu_i^s = \sum_{j\neq i} u_{\alpha\beta}(r_{ij})\, r_{ij}^s \qquad \lambda_i^{st} = \sum_{j\neq i} w_{\alpha\beta}(r_{ij})\, r_{ij}^s r_{ij}^t \qquad \nu_i = \sum_s \lambda_i^{ss}$$

NP is created in cylindrical shape. Radius is equal to 20 and 40 nm, thickness is 10 nm. Aluminum is printed as blue and silicon grain structure color is grey. Gold color is yellow.

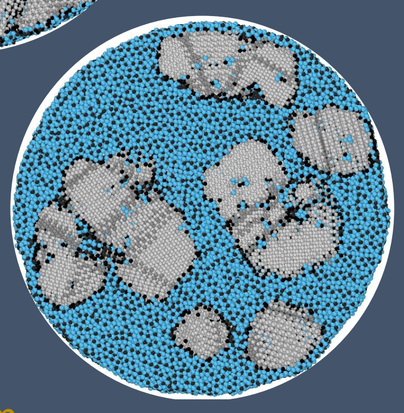
Ø 40 nm
20% of Al



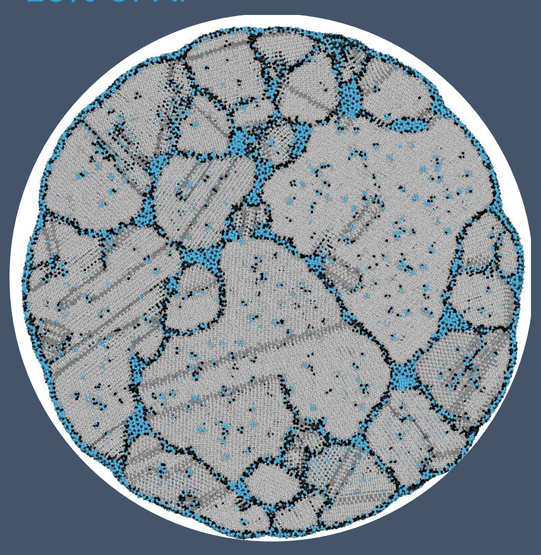


Ø 40 nm
10% of Al

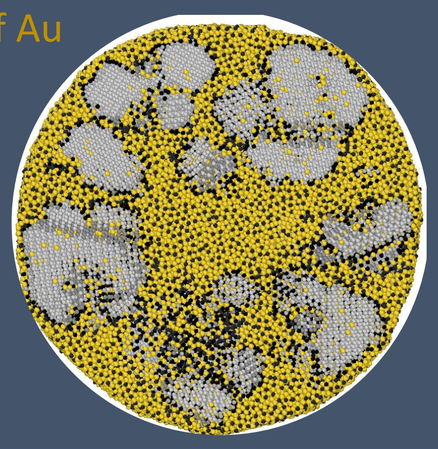
Ø 40 nm
40% of Al



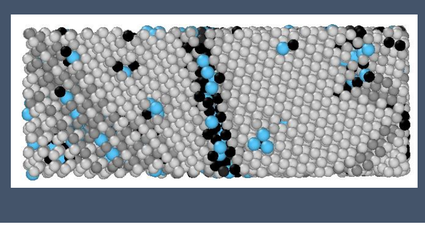
Ø 80 nm
10% of Al

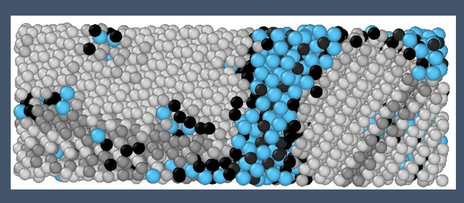


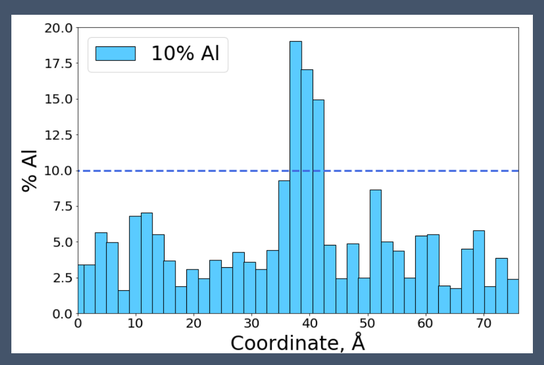
Ø 40 nm
25% of Au

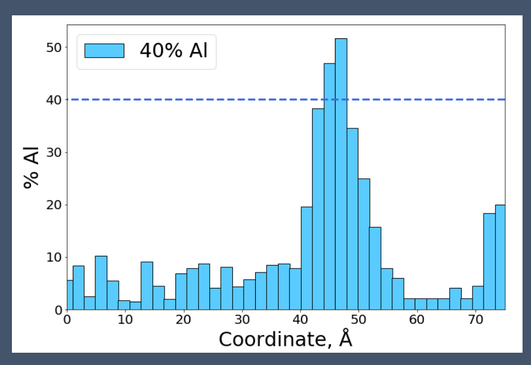


Results

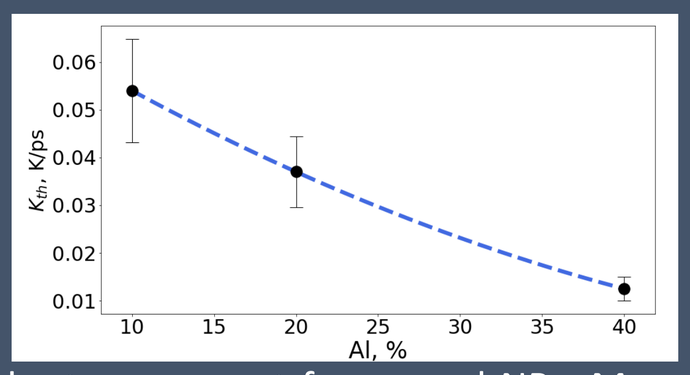








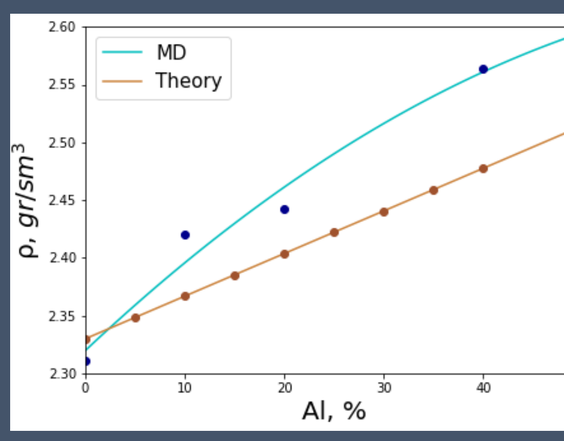
The images show the grain structure and distribution of Al.

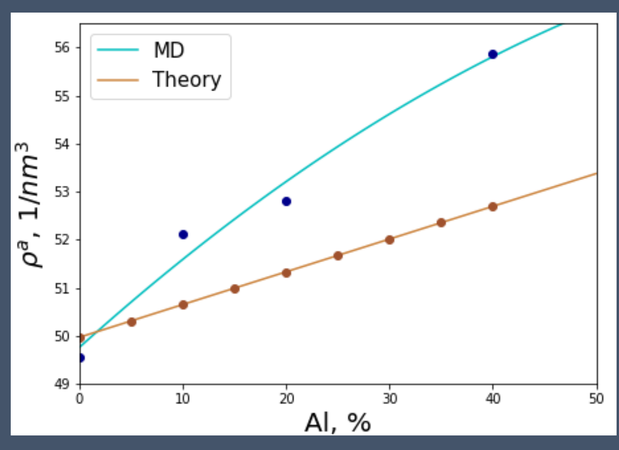


The threshold rates were got for several NPs. Moreover, molecular dynamics showed different meanings for density and atomic density of NPs, because they depend on volume of particle.

$$\rho_{np} = \frac{N_{Si}\cdot m_{Si} + N_{Al}\cdot m_{Al}}{V_{np}}$$

$$\rho_{np}^a = \frac{N_{Al} + N_{Si}}{V_{np}}$$

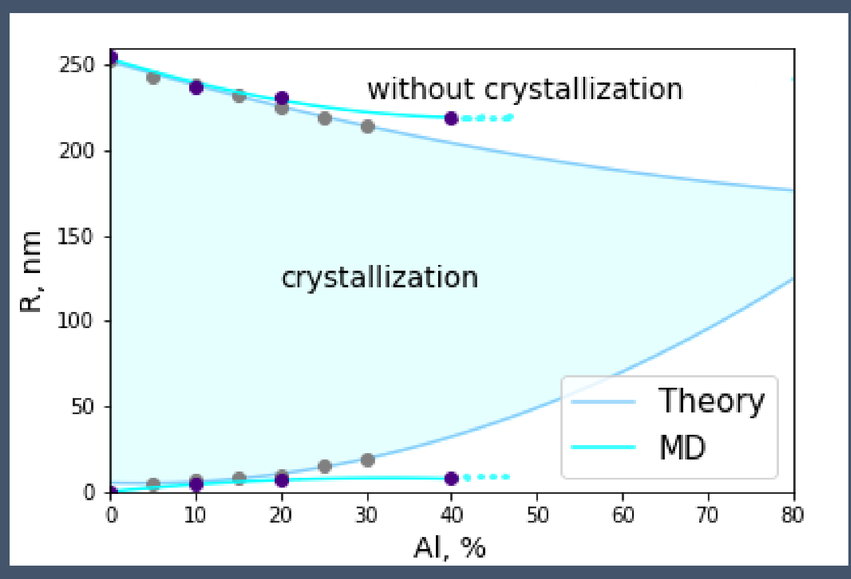




In that study it is possible to get allowed sizes for NPs, if threshold rates are known.

$$R_{up}^2 \approx R_0^2 \cdot \frac{\rho_{Si}}{\rho_{np}} \cdot \left(1 - \exp\left(\frac{0{,}75T_{liq} - T_0}{\alpha_\rho t_R R_{up}}\right)\right)^{-1}$$

$$R_{down} \approx 50 \cdot \frac{K_0}{K_{th}} \cdot \frac{\rho_{Si}^a}{\rho_{np}^a}$$



Conclusions

- Simulations of nanoparticles in wide range of concentrations of Al was carried out.
- Dependence of threshold rate on quantity of Al was obtained.
- The physical parameters of NP have been received from molecular dynamics were studied.