Molecular dynamics study of the glass transition temperature and elastic properties of the Zr-Nb amorphous alloy

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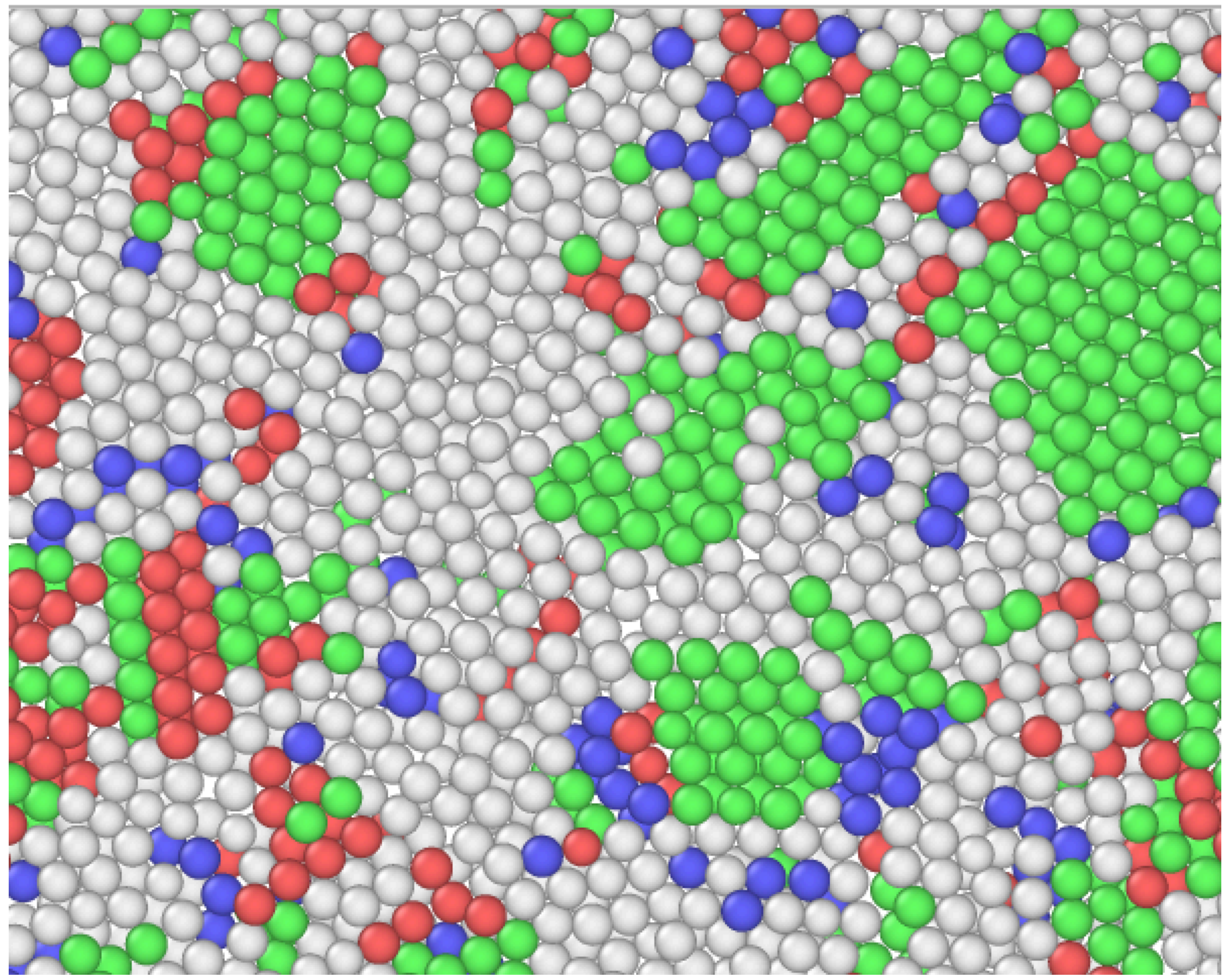
EPFL, JIHT RAS

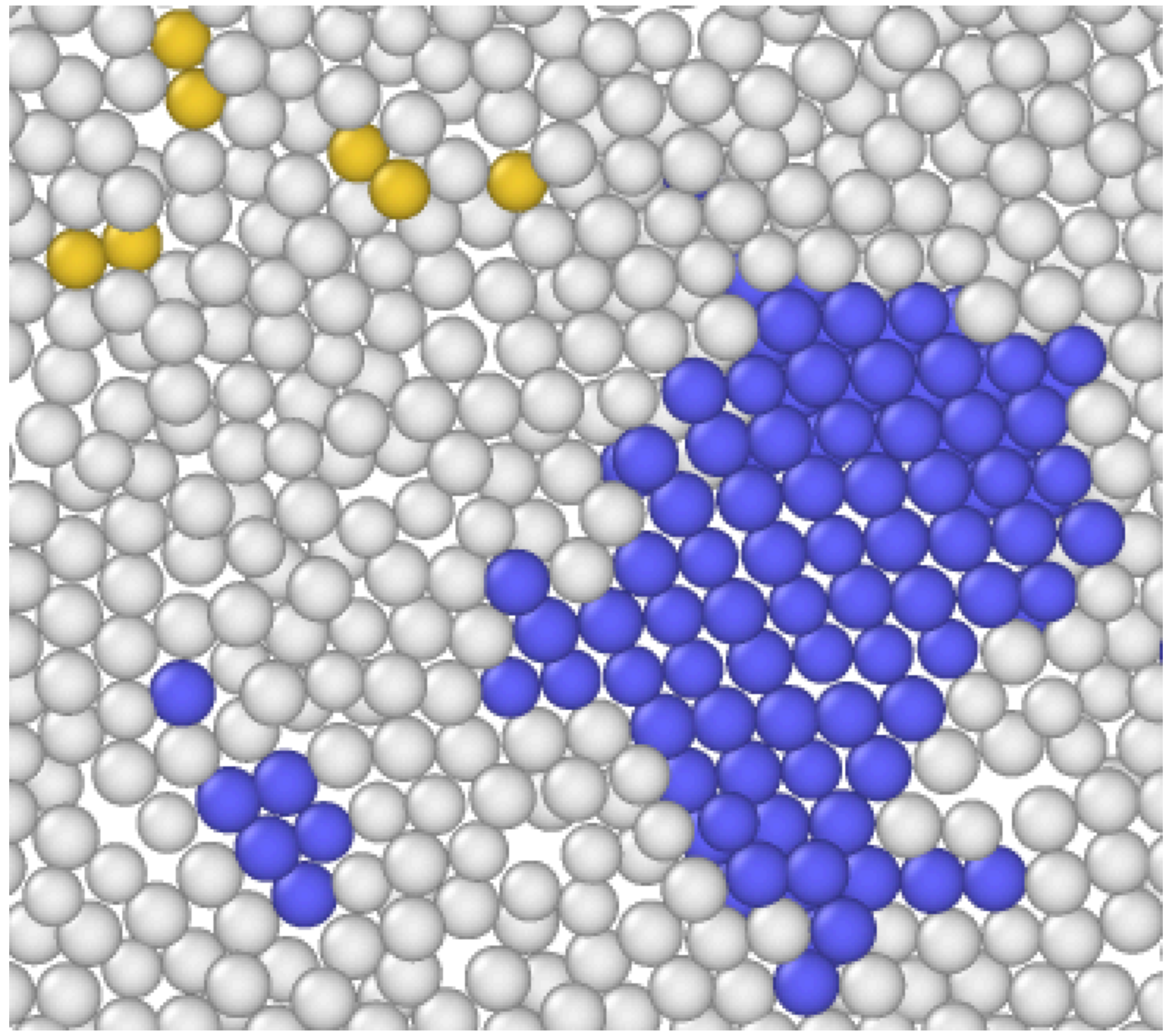
IIEFM 2021

Research motivation

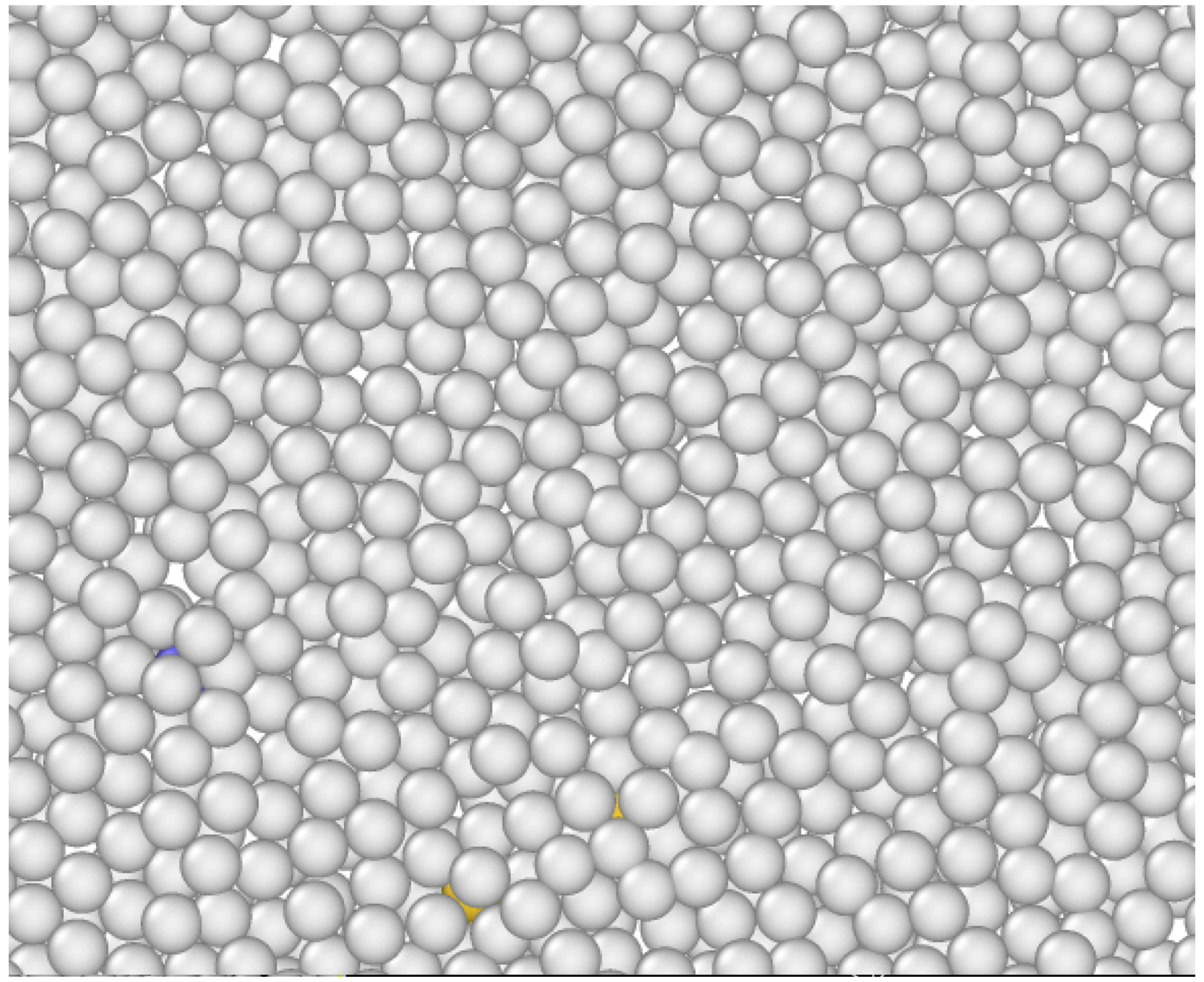
Research motivation



Nanocrystalline alloy



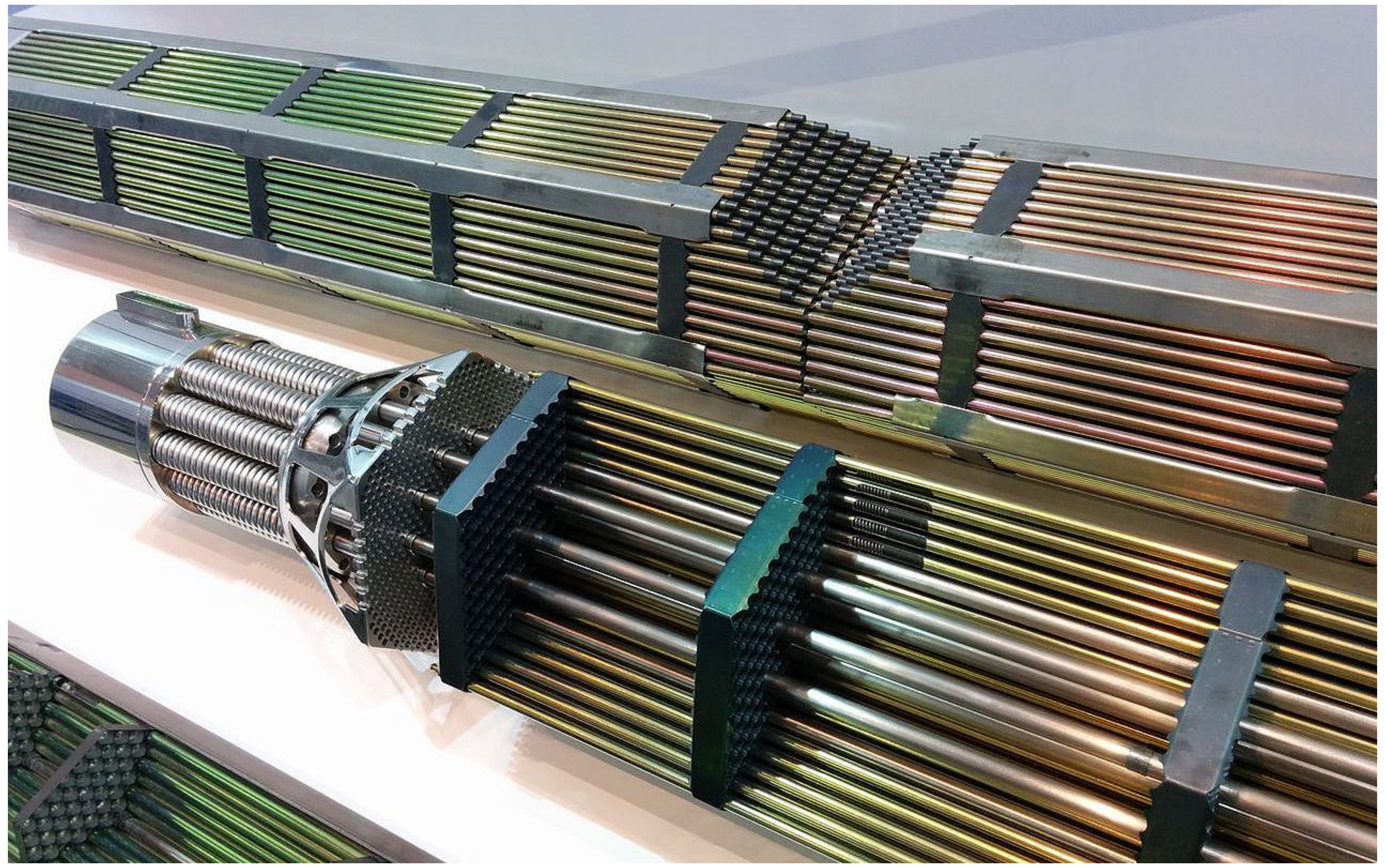
Transitional state (crystalline nuclei in the amorphous phase)



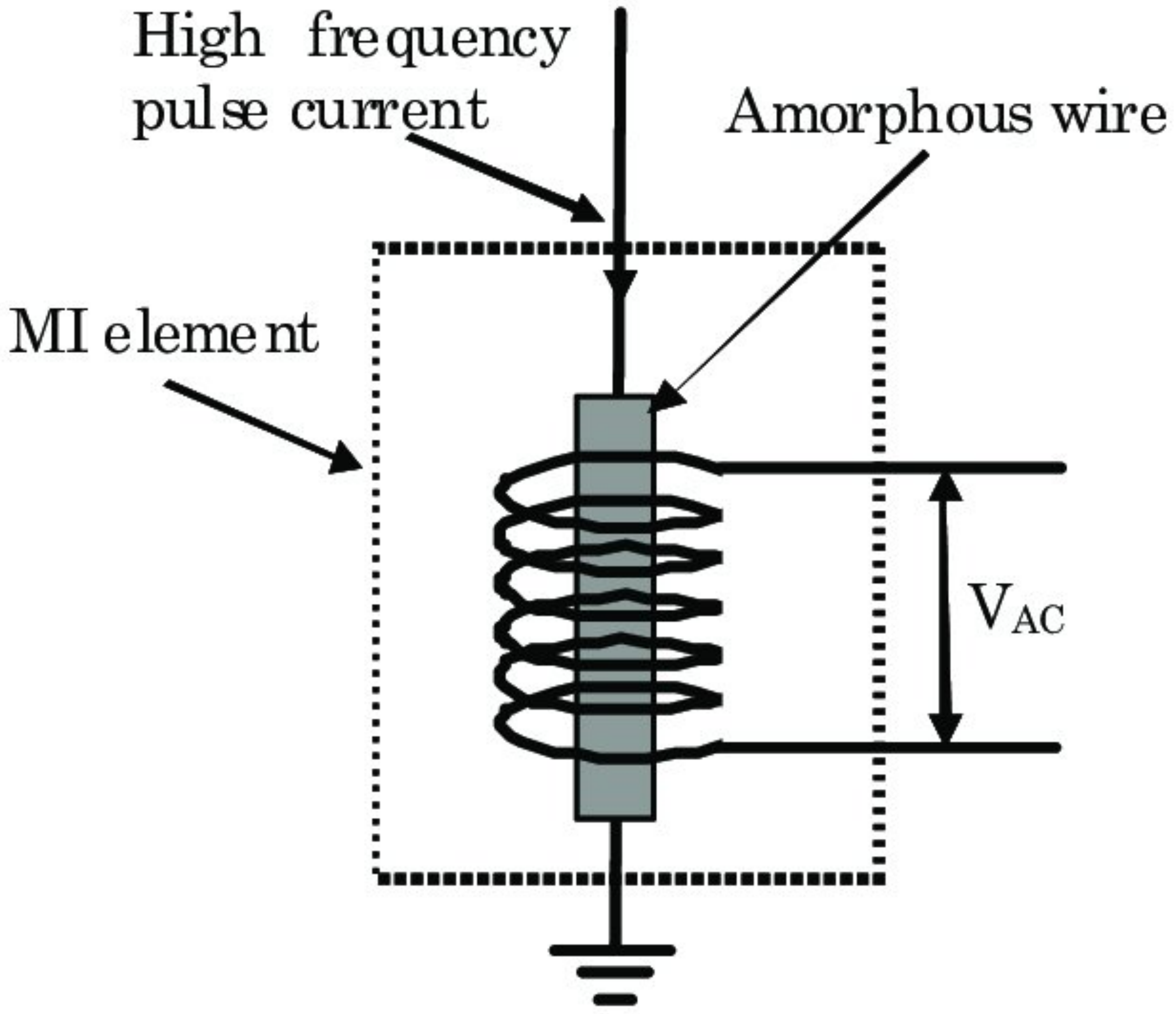
Amorphous phase

Research motivation

Fuel element shell



Magnetic sensors



D. He, MDPI (2020).

Structure and structural criteria Zr-Nb:

Kliavinek S., Kolotova L., JETP (2020).

Molecular dynamics model

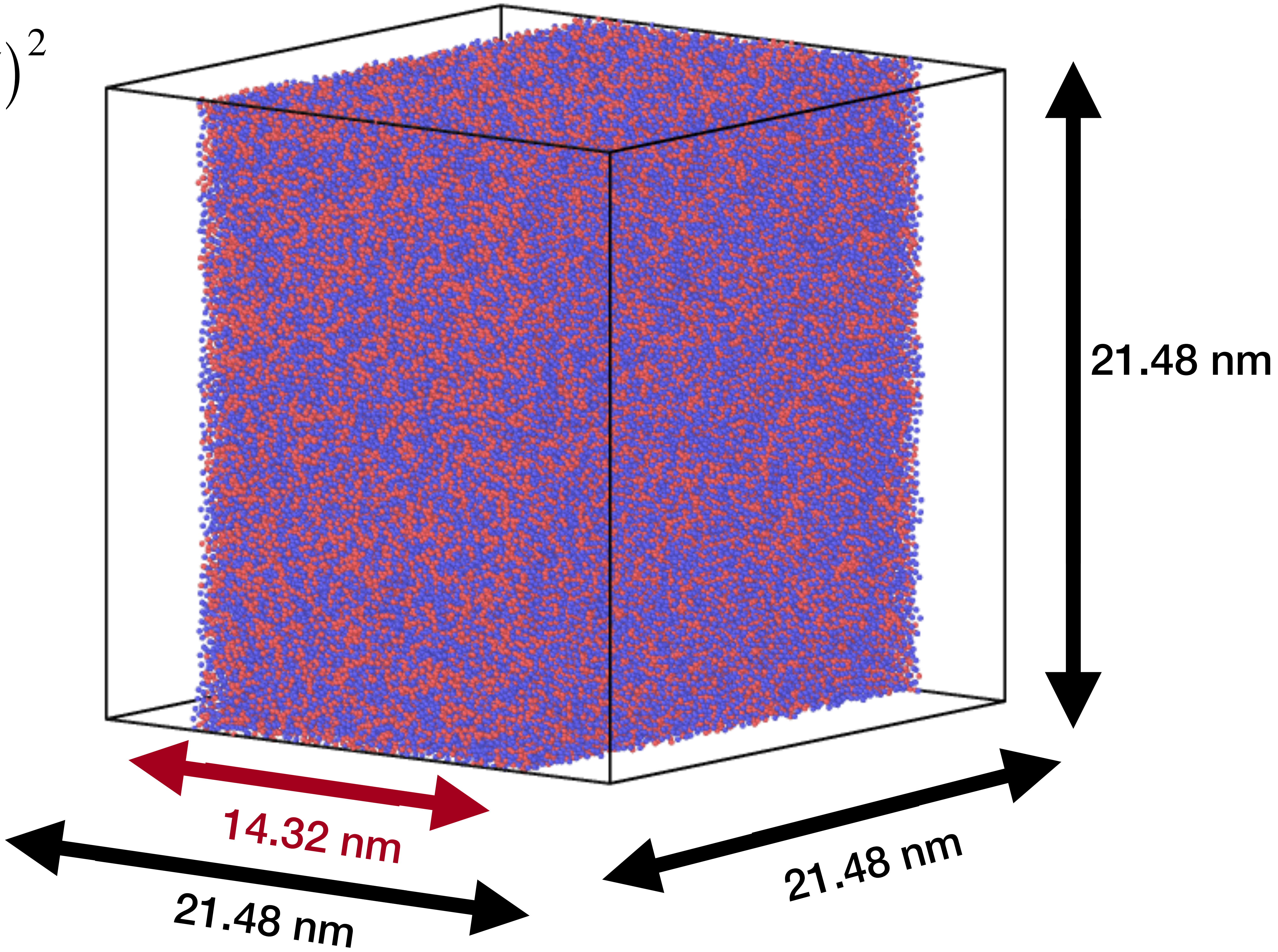
Molecular dynamics model

$$E_{\text{tot}} = \frac{1}{2}\sum_{i,j(j\neq i)} \Phi_{s_i s_j}\left(r_{ij}\right) + \sum_i F_{s_i}\left(\bar{\rho}_i\right) + \frac{1}{2}\sum_{i,\alpha}\left(\mu_i^{\alpha}\right)^2 + \frac{1}{2}\sum_{i,\alpha,\beta}\left(\lambda_i^{\alpha\beta}\right)^2 - \frac{1}{6}\sum_i v_i^2$$

ADP-potential (Zr-Nb, Smirnova, Starikov, 2017)

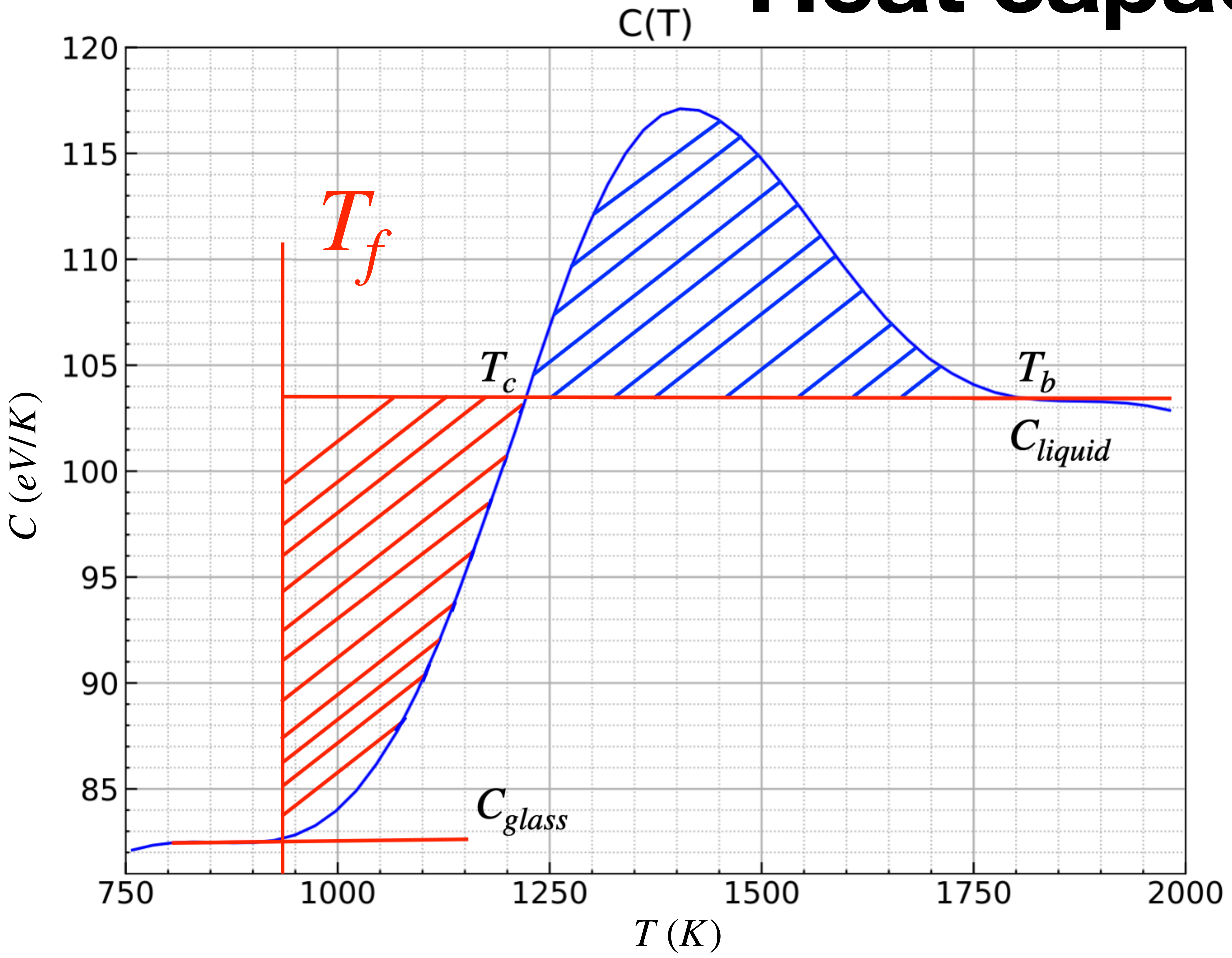
Nb: 25-75%
K: 11 K/ps

Glass transition temperature was determined on heating



Glass transition temperature

Heat capacity



$$C = \frac{\delta H}{\delta T}$$

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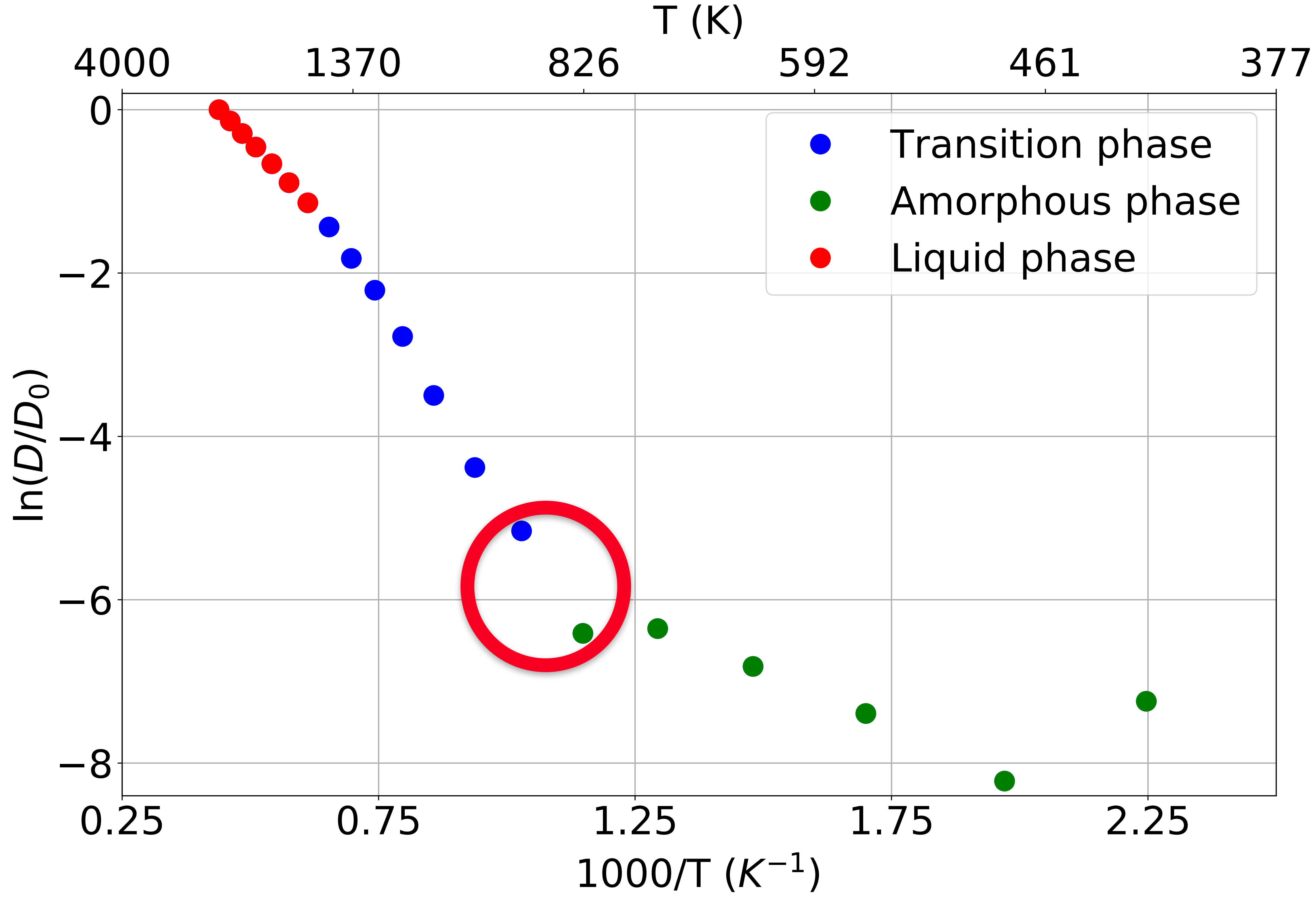
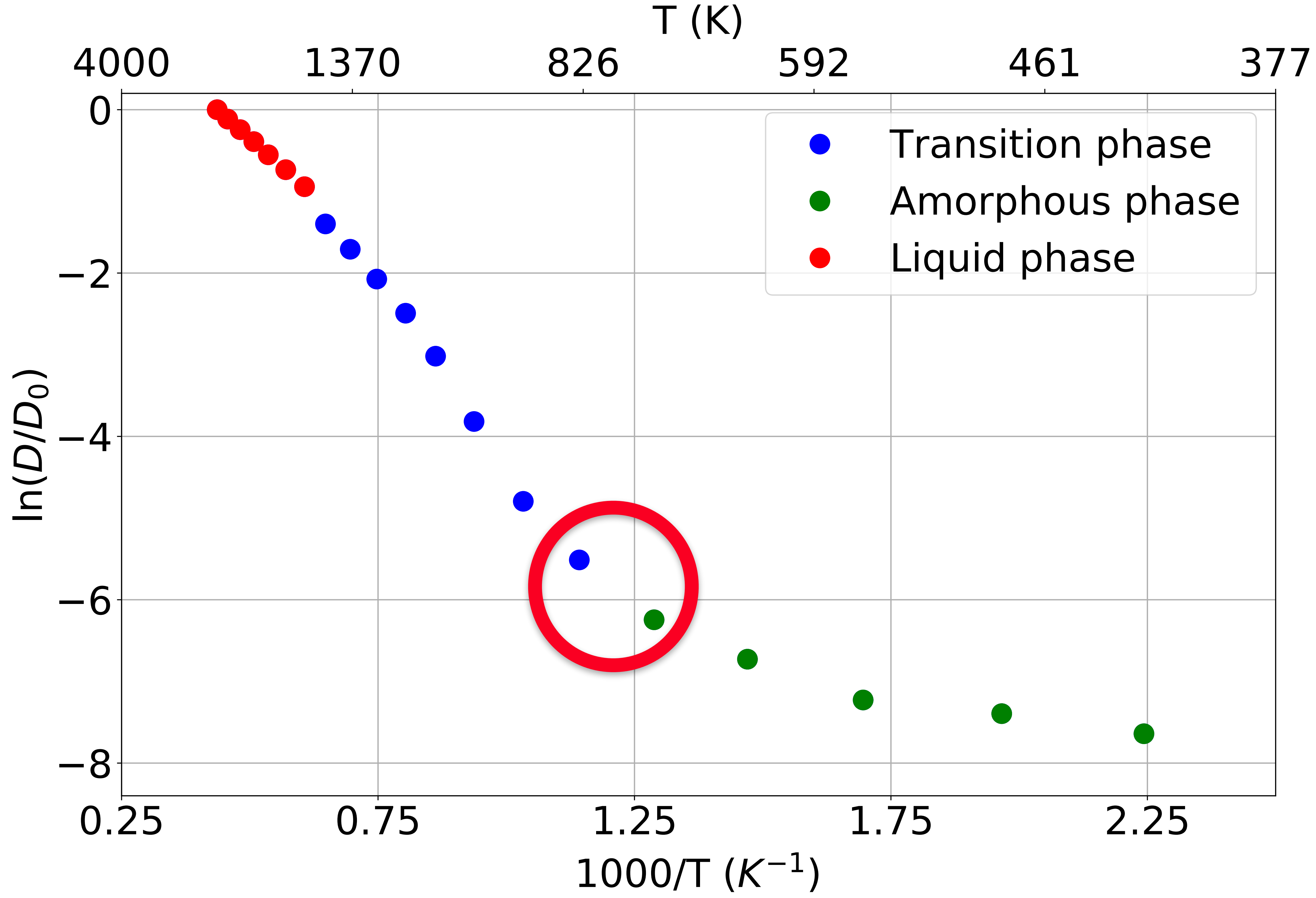
Diffusion coefficient

$$< r^2 > = < r_0^2 > + 6Dt$$



50% Nb



30% Nb

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Viscosity coefficient

$$\eta = \lim_{t\to\infty} \frac{V}{kT} \int_0^t < P_{\gamma\varepsilon}(0) P_{\gamma\varepsilon}(\tau) > d\tau$$

↓

$$\int_0^t < P_{\gamma\varepsilon}(0) P_{\gamma\varepsilon}(\tau) > d\tau = A \exp^{(-t/T)} + B$$

↓

$$\eta = \eta_0 \exp\left(\frac{E}{k(T+T_0)}\right)$$

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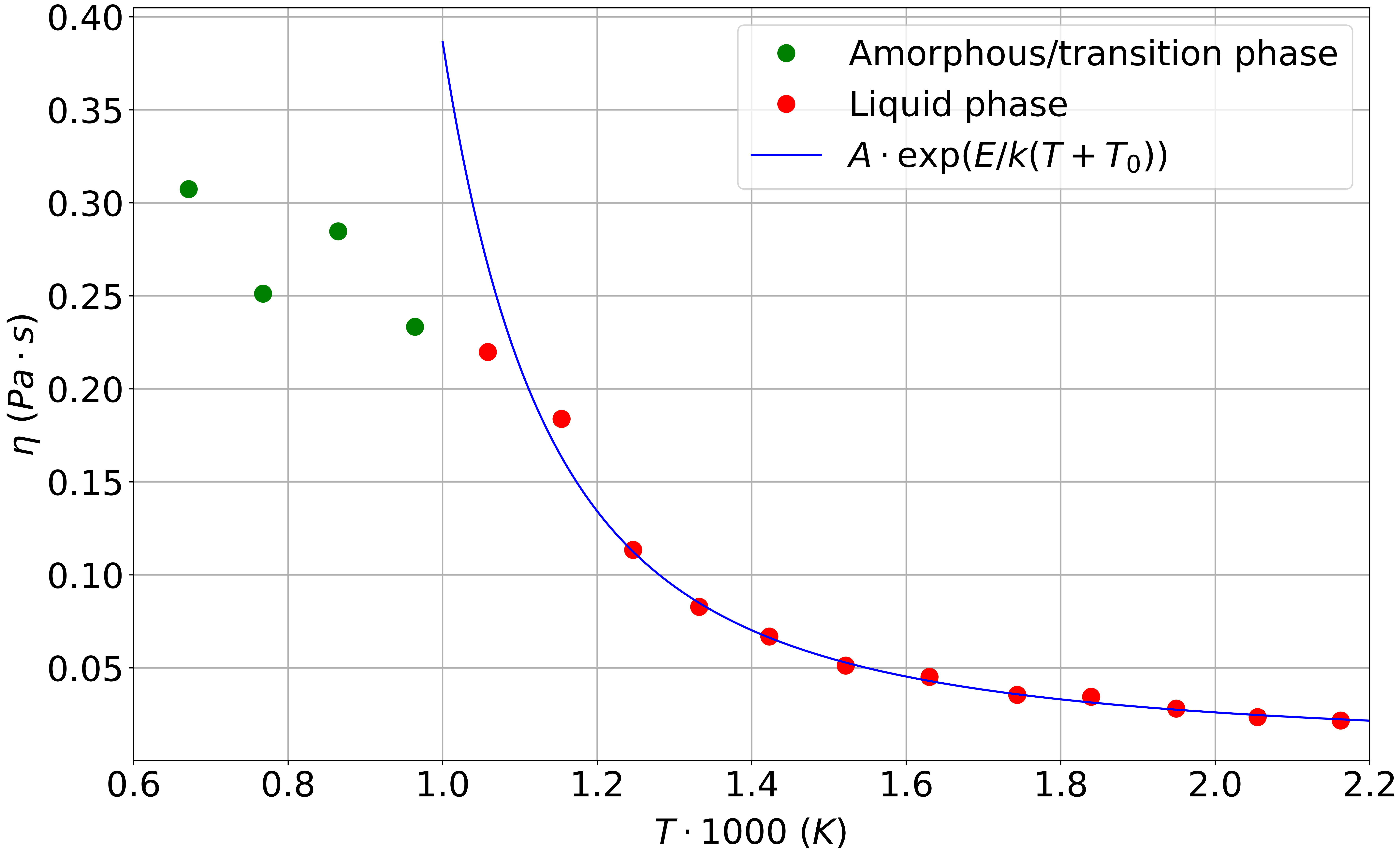
Viscosity coefficient



45% Nb

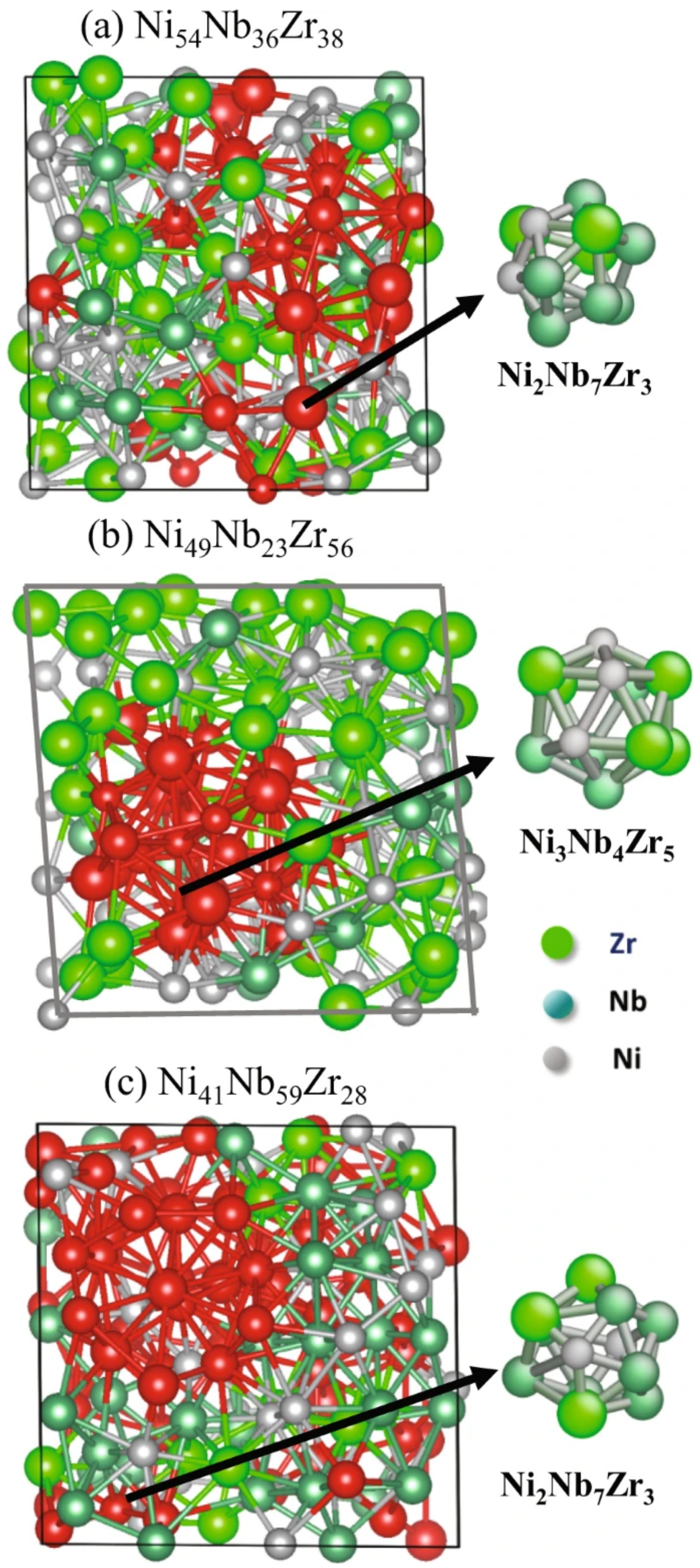
Glass transition temperature

T_g (K)	
Heat capacity	900
Diffusion coefficients	900
Viscosity coefficient	1000

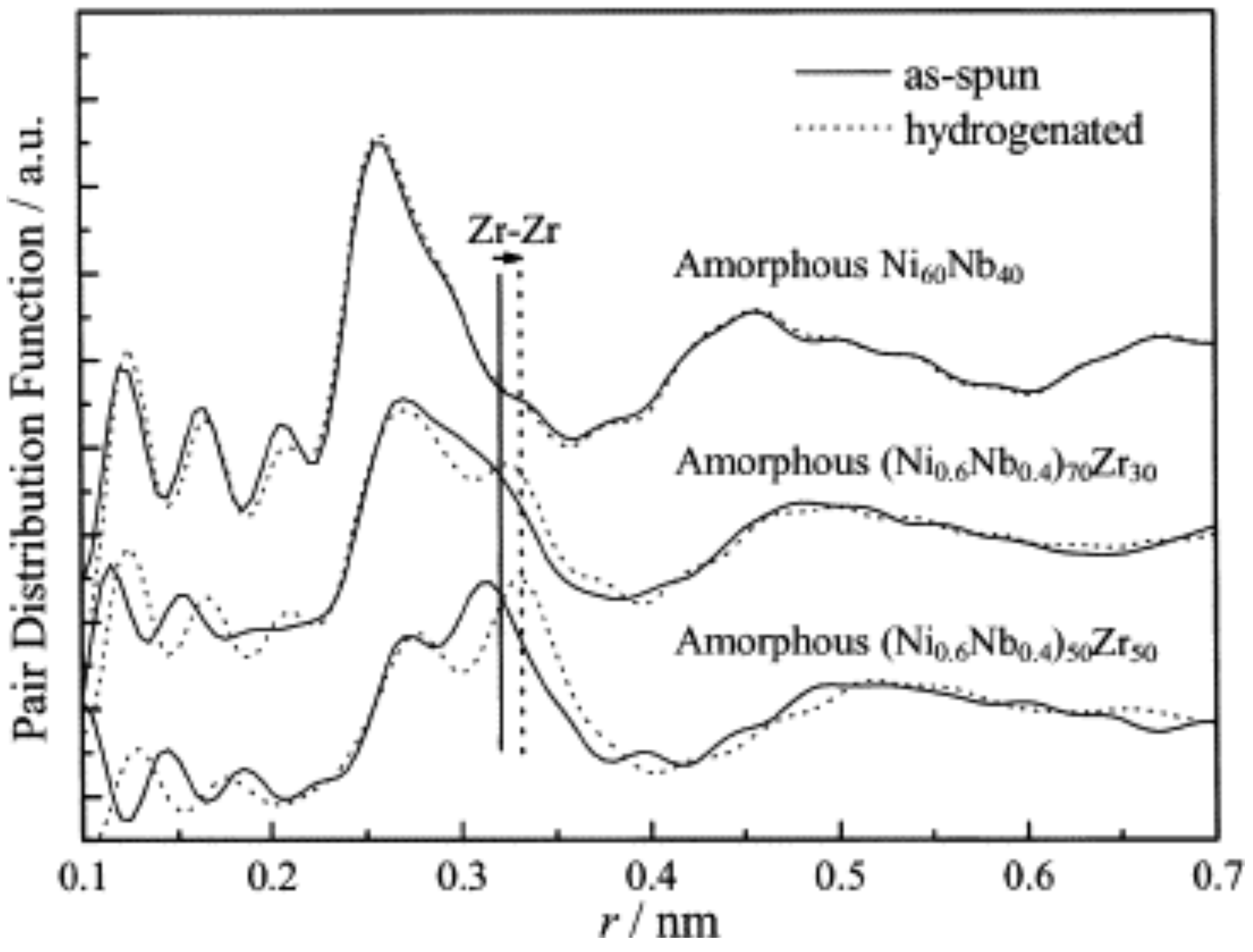
T_g (K)	
Square under second peak	1050
Vendt-Abraham	1200
Icosahedral clusters	1200

50% Nb

Glass transition temperature

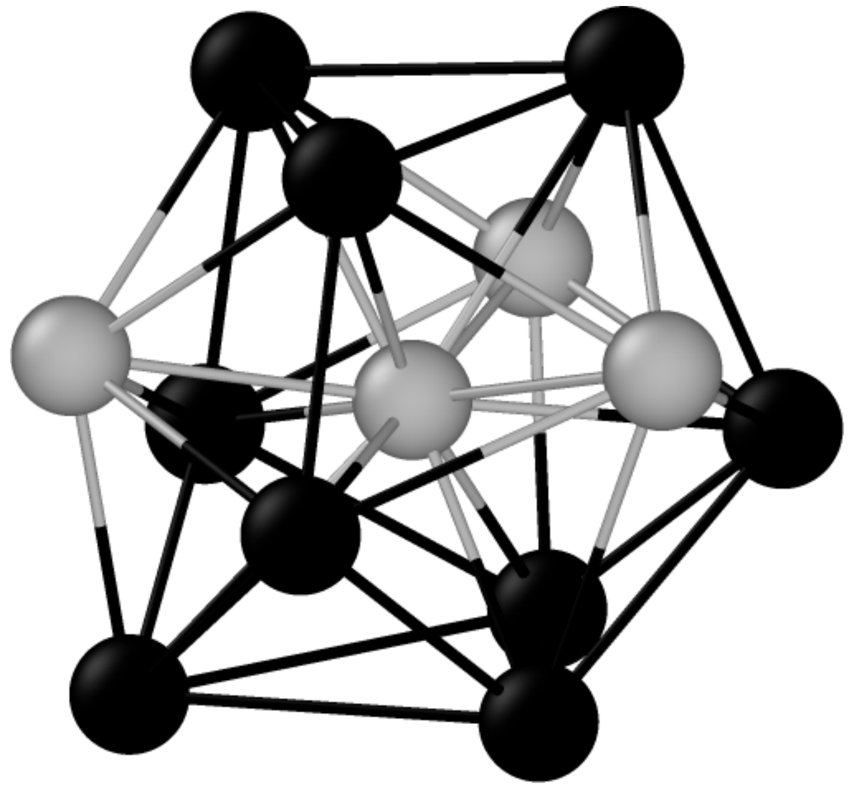


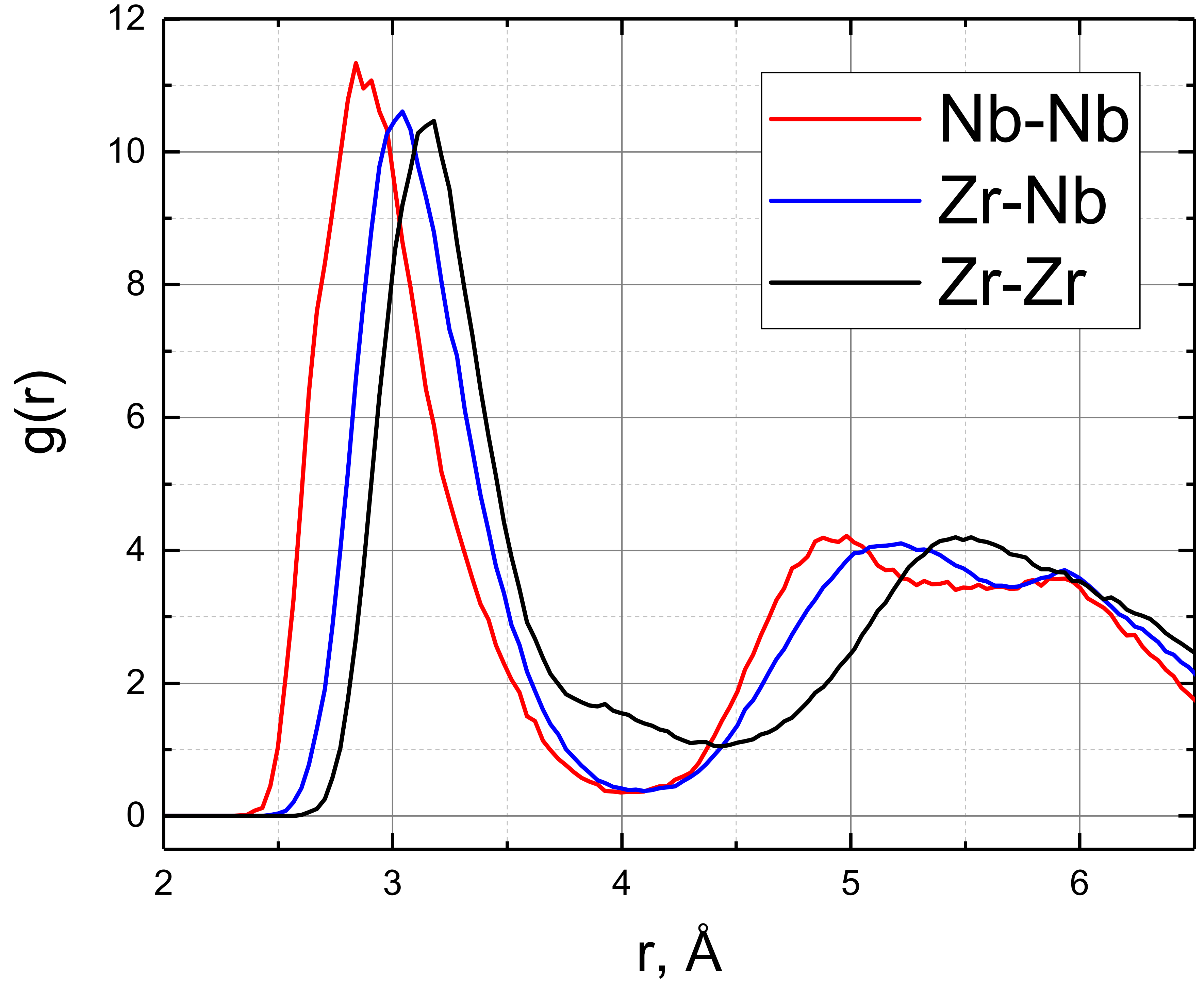
Sarker S. et al, Scientific reports (2018)



Yamaura S. et al., Acta Materialia (2005)

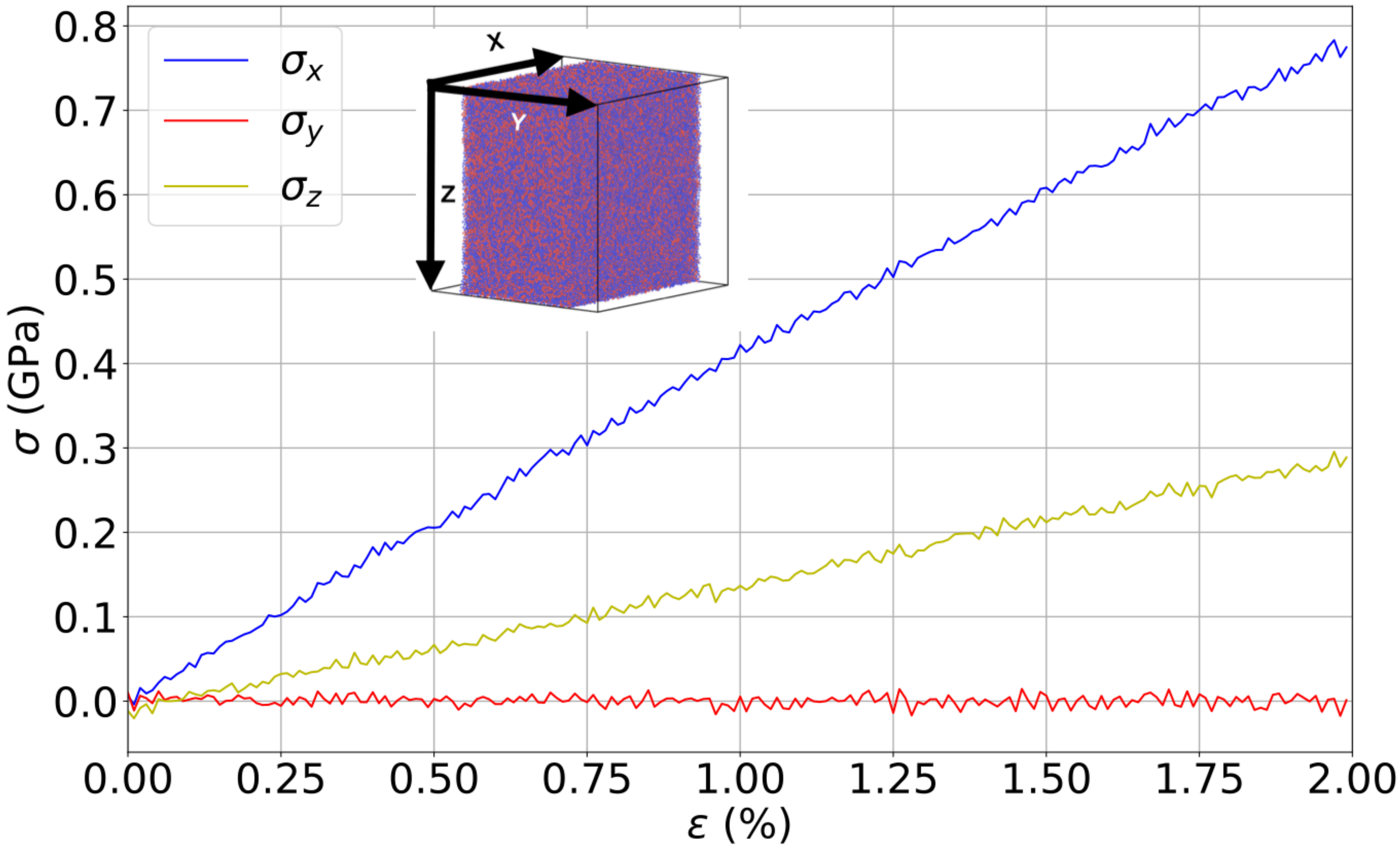
Kliavinek S., Kolotova L., JETP (2020).





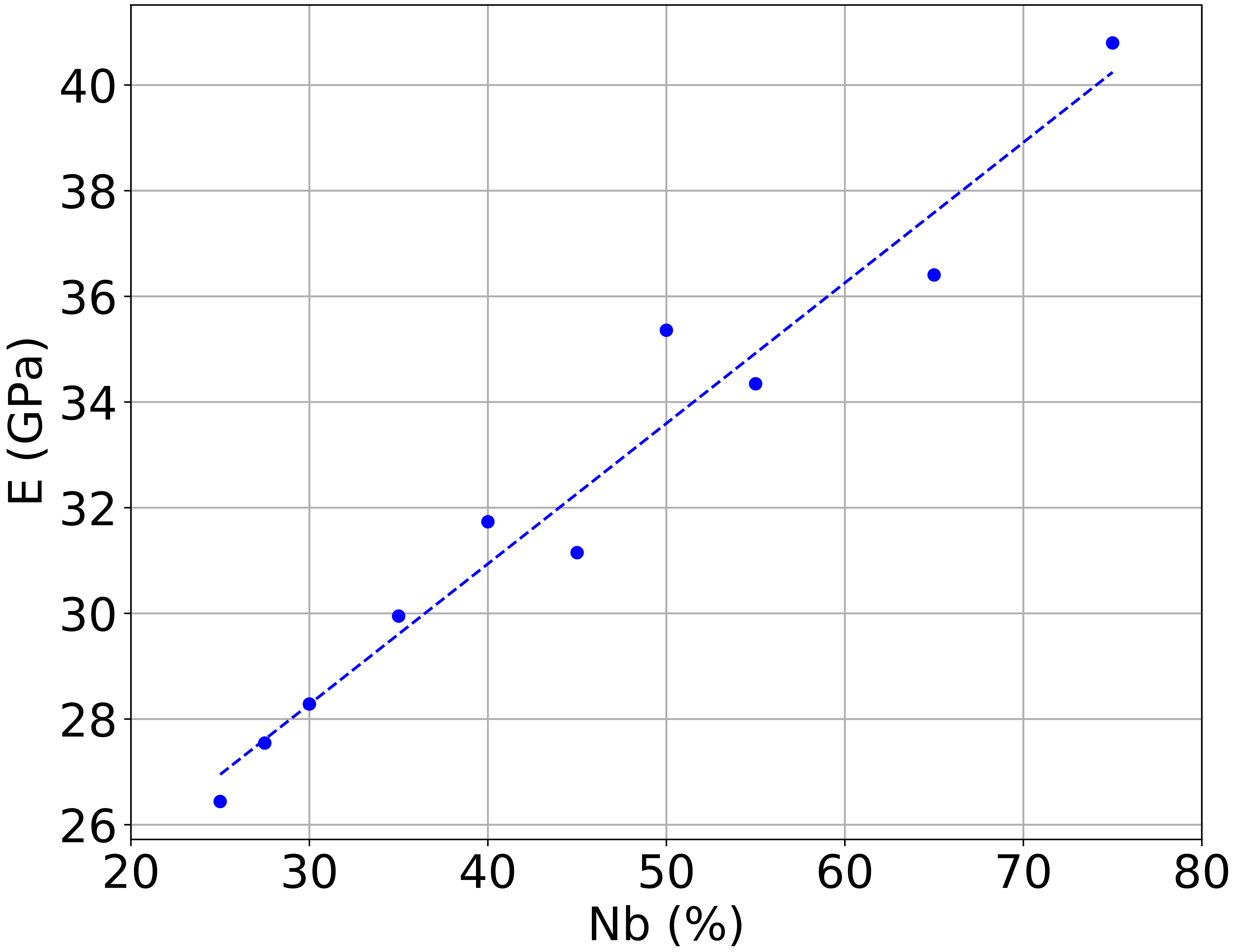
Elastic properties

Young modulus



50% Nb

Young modulus



For crystalline Zr-Nb $E \approx 100$ GPa

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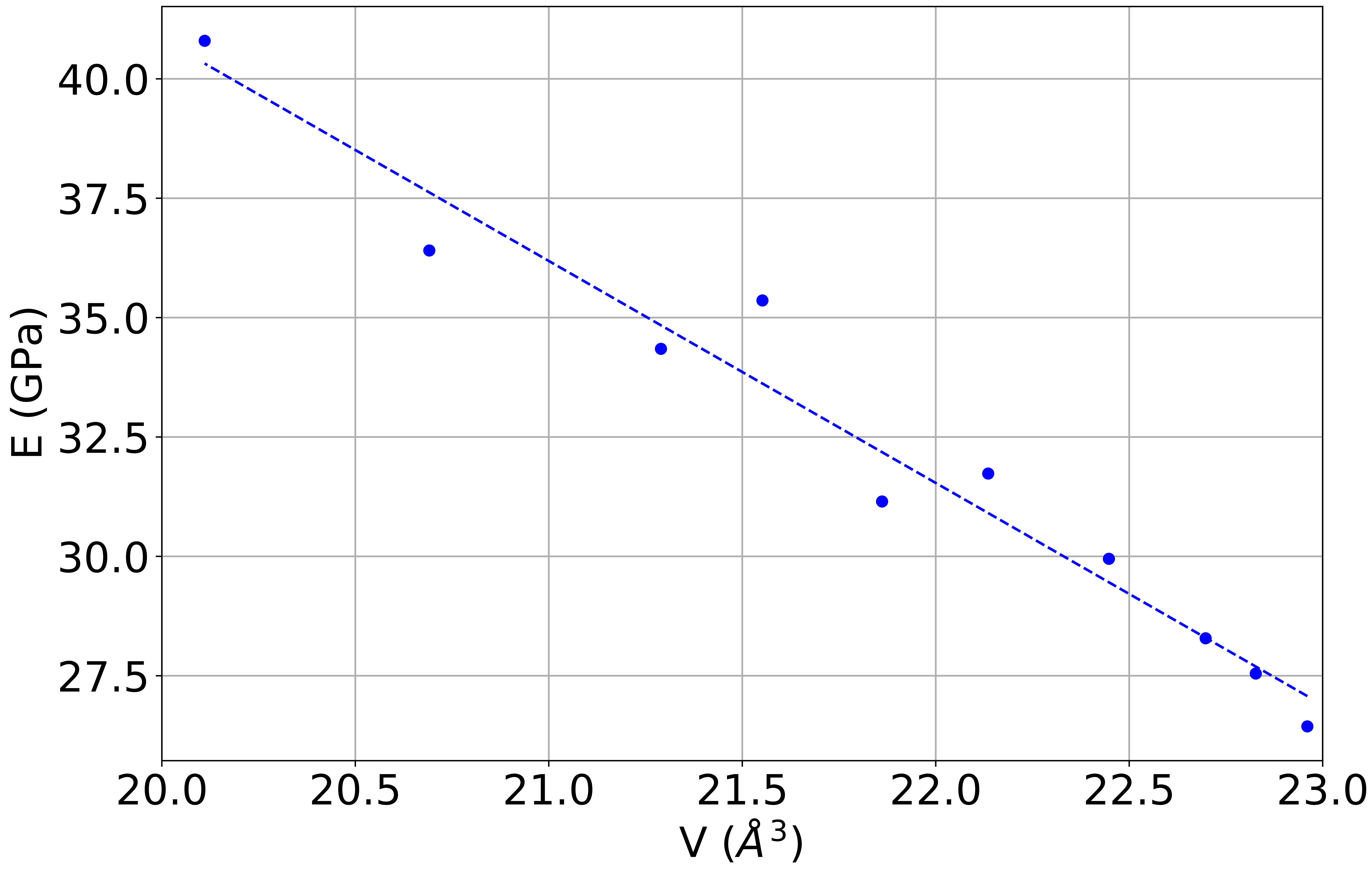
Young modulus



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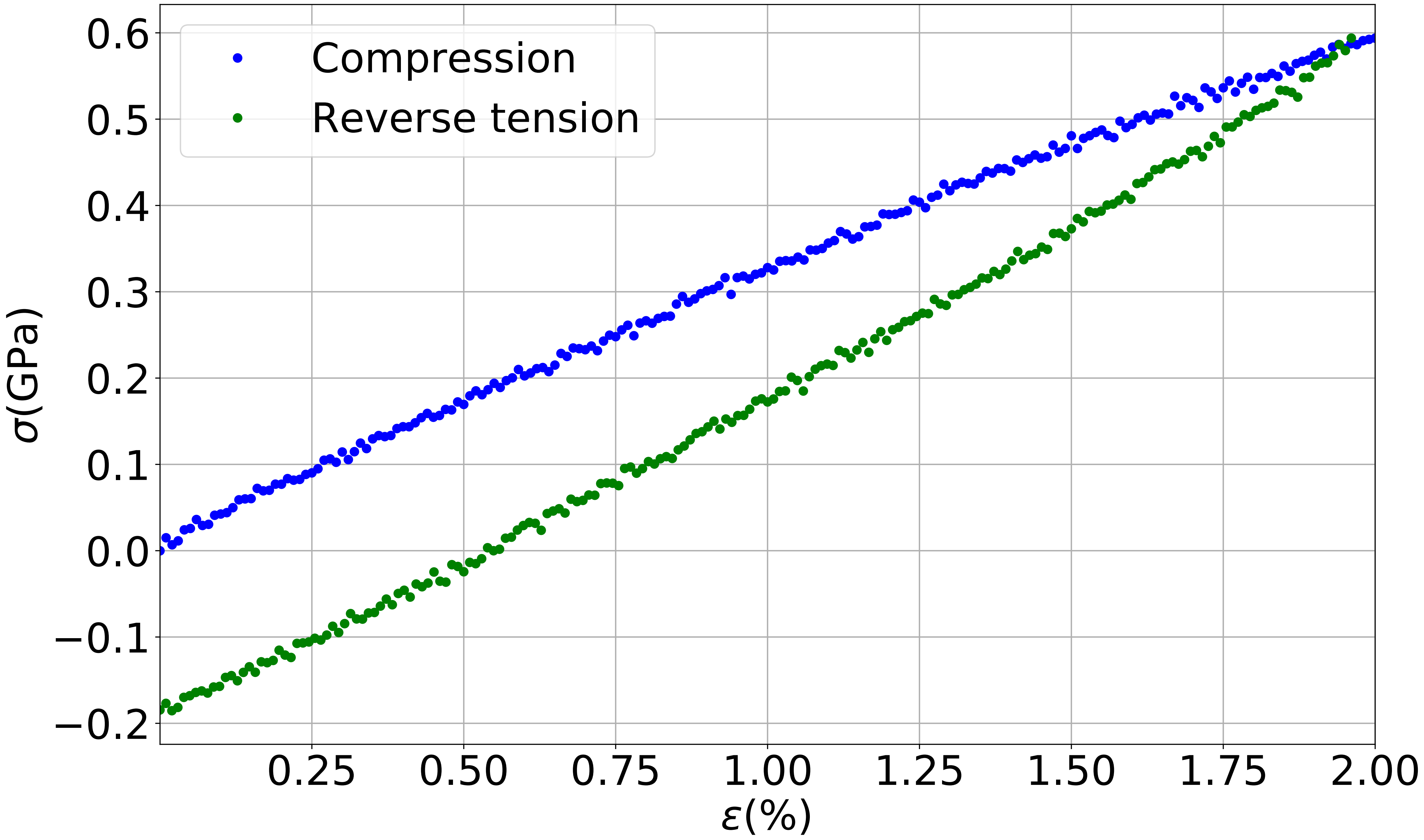
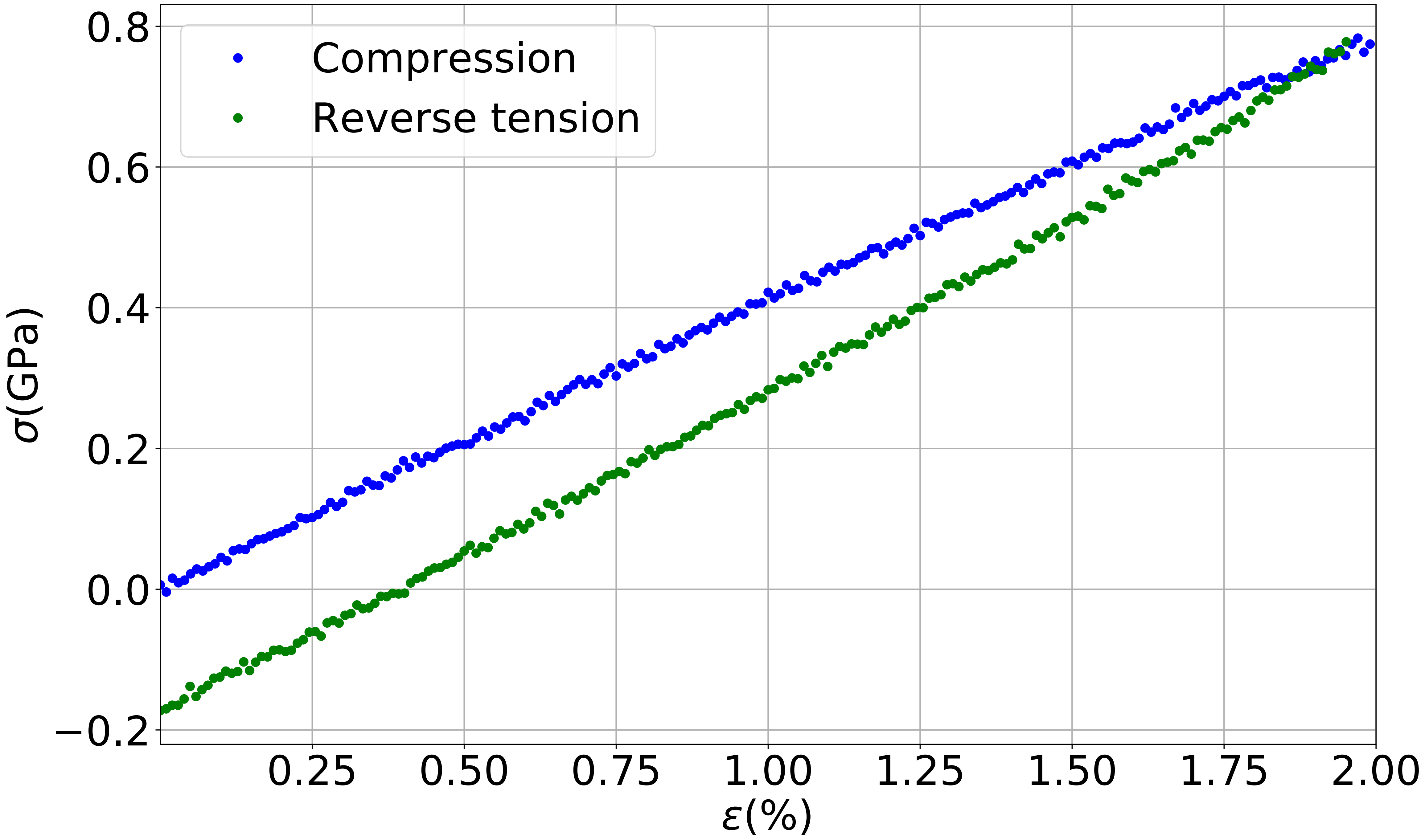
Deformation hysteresis

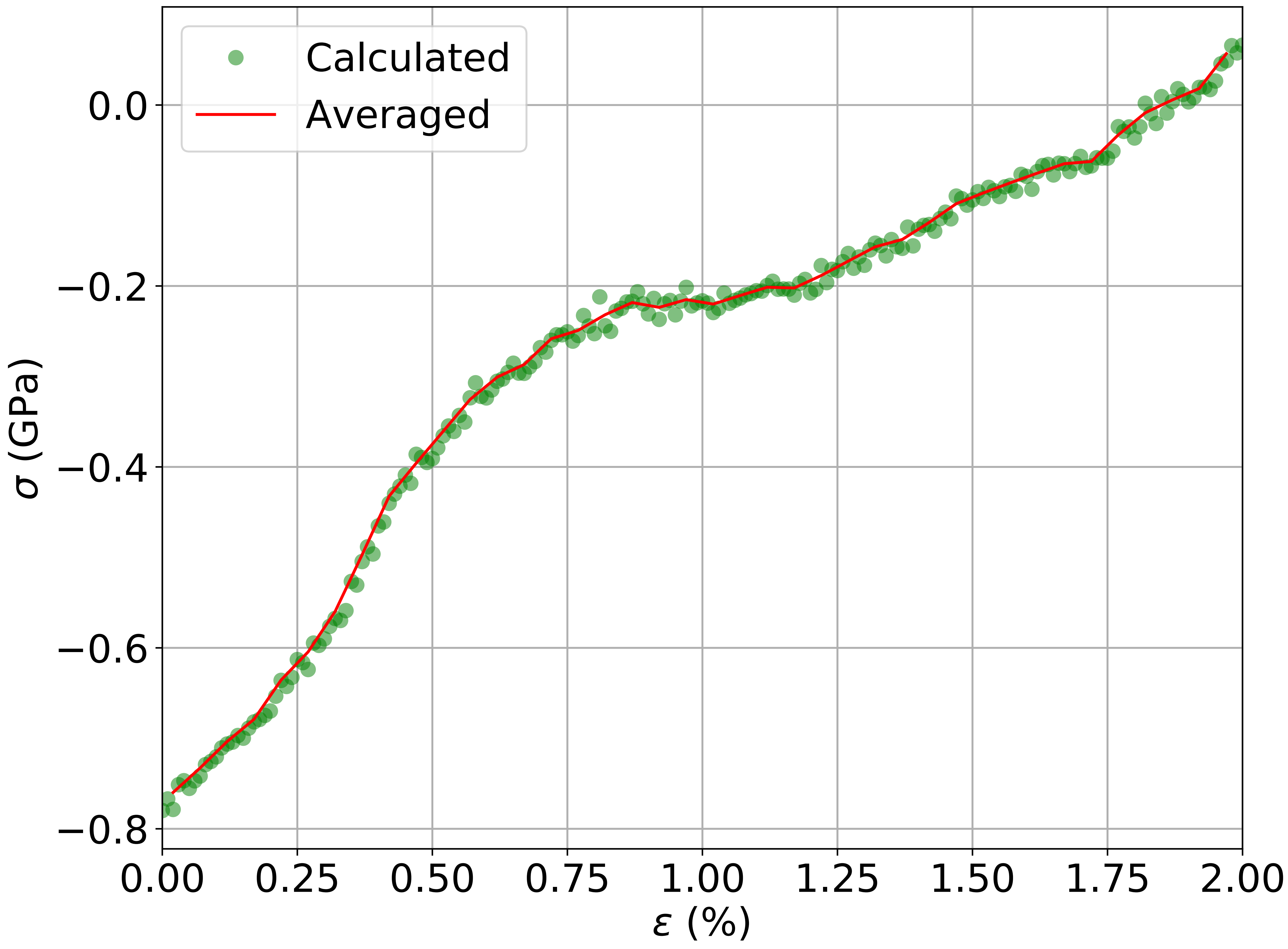


25% Nb



75% Nb

Tensile crystallization



50% Nb

$T \approx 1000$ K

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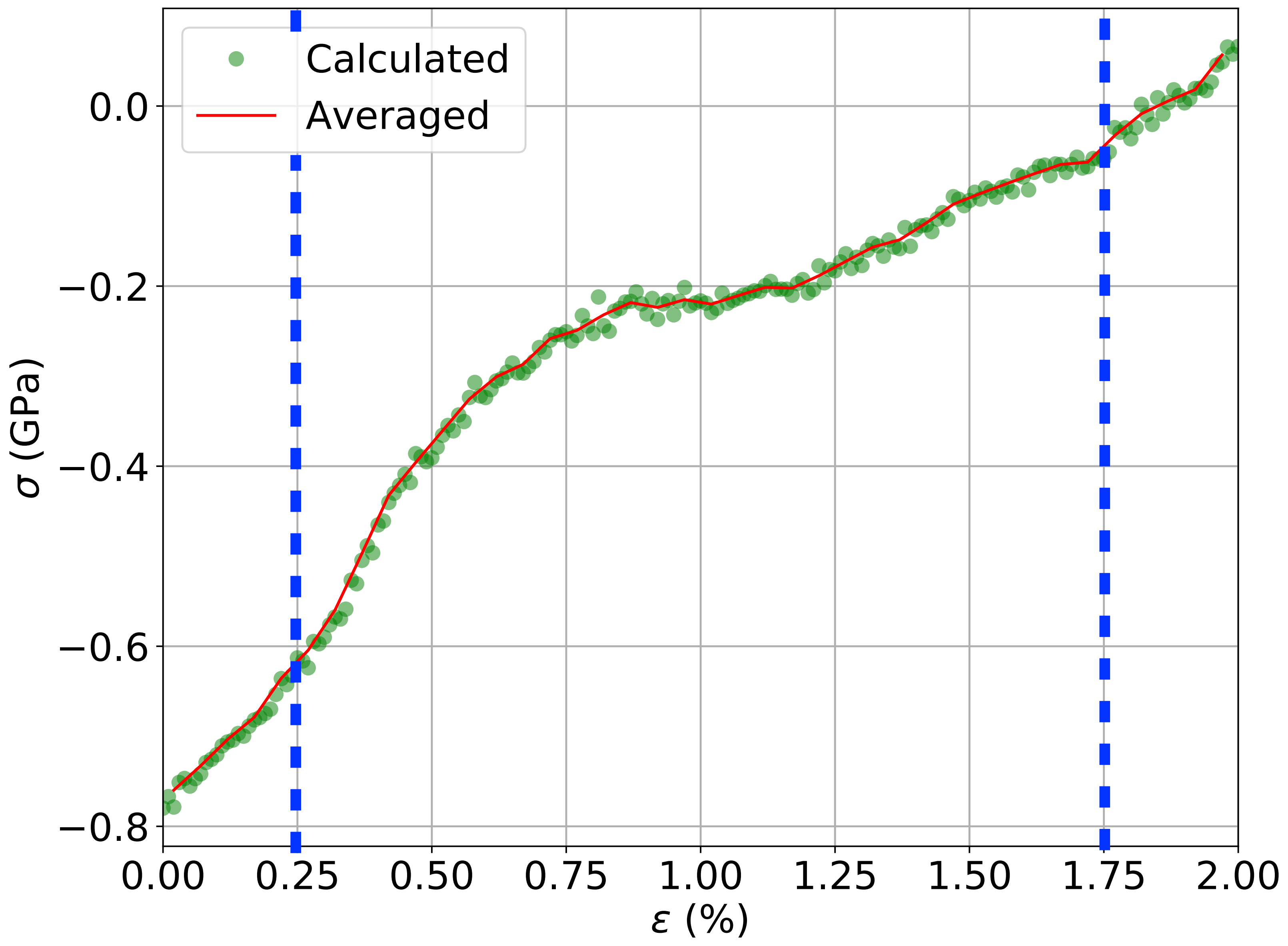
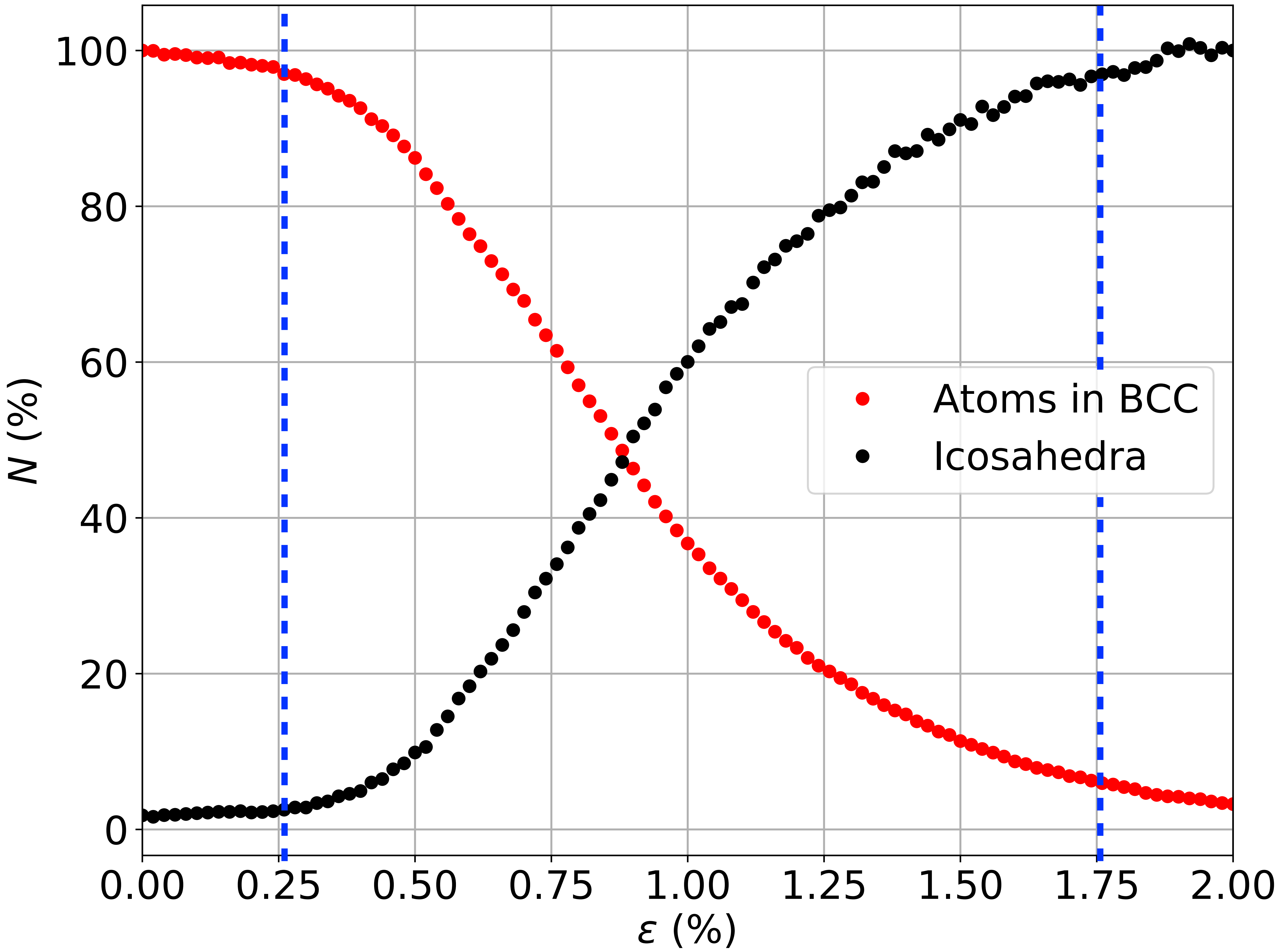
Tensile crystallization

50% Nb $T \approx 1000$ K





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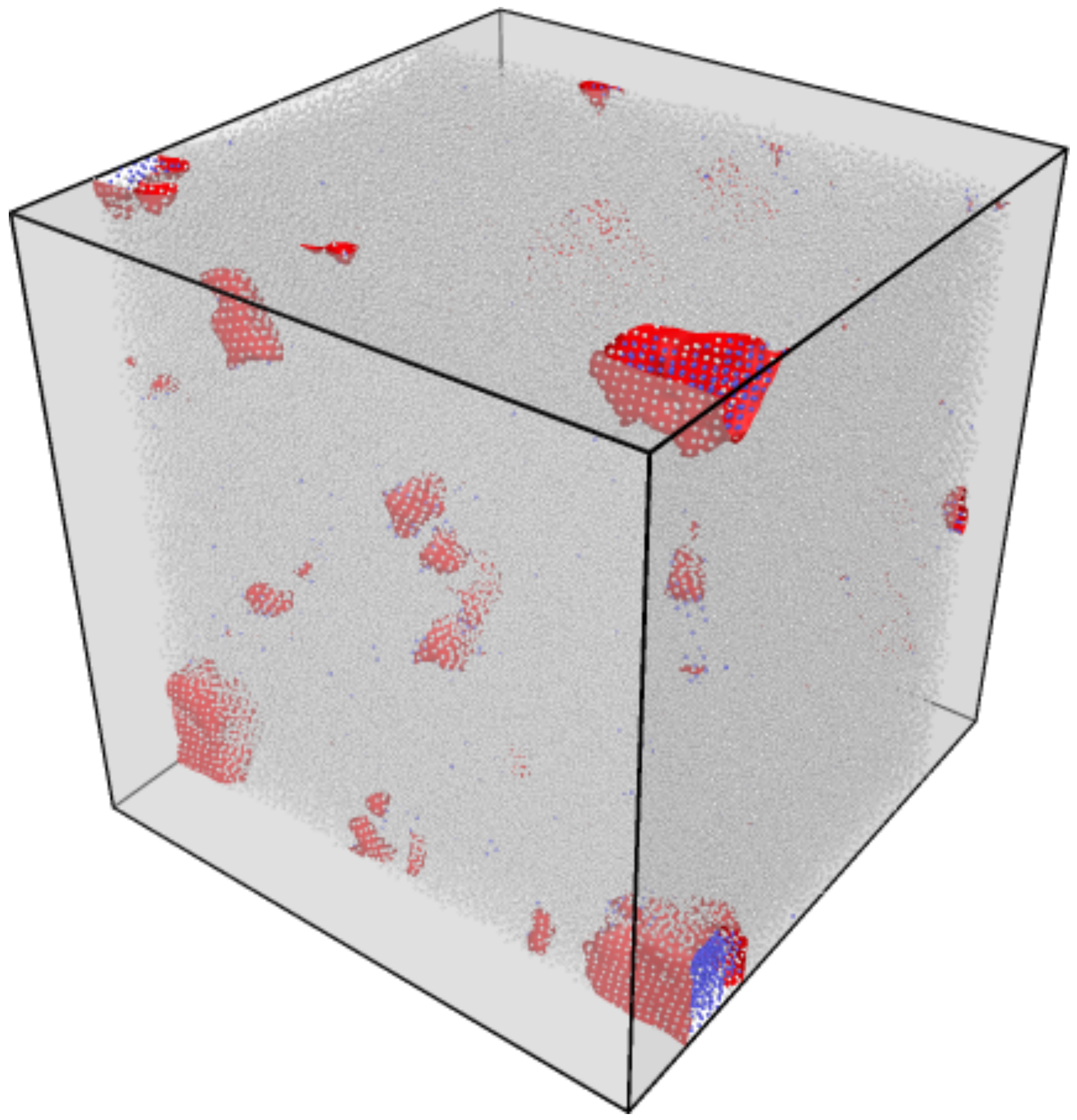
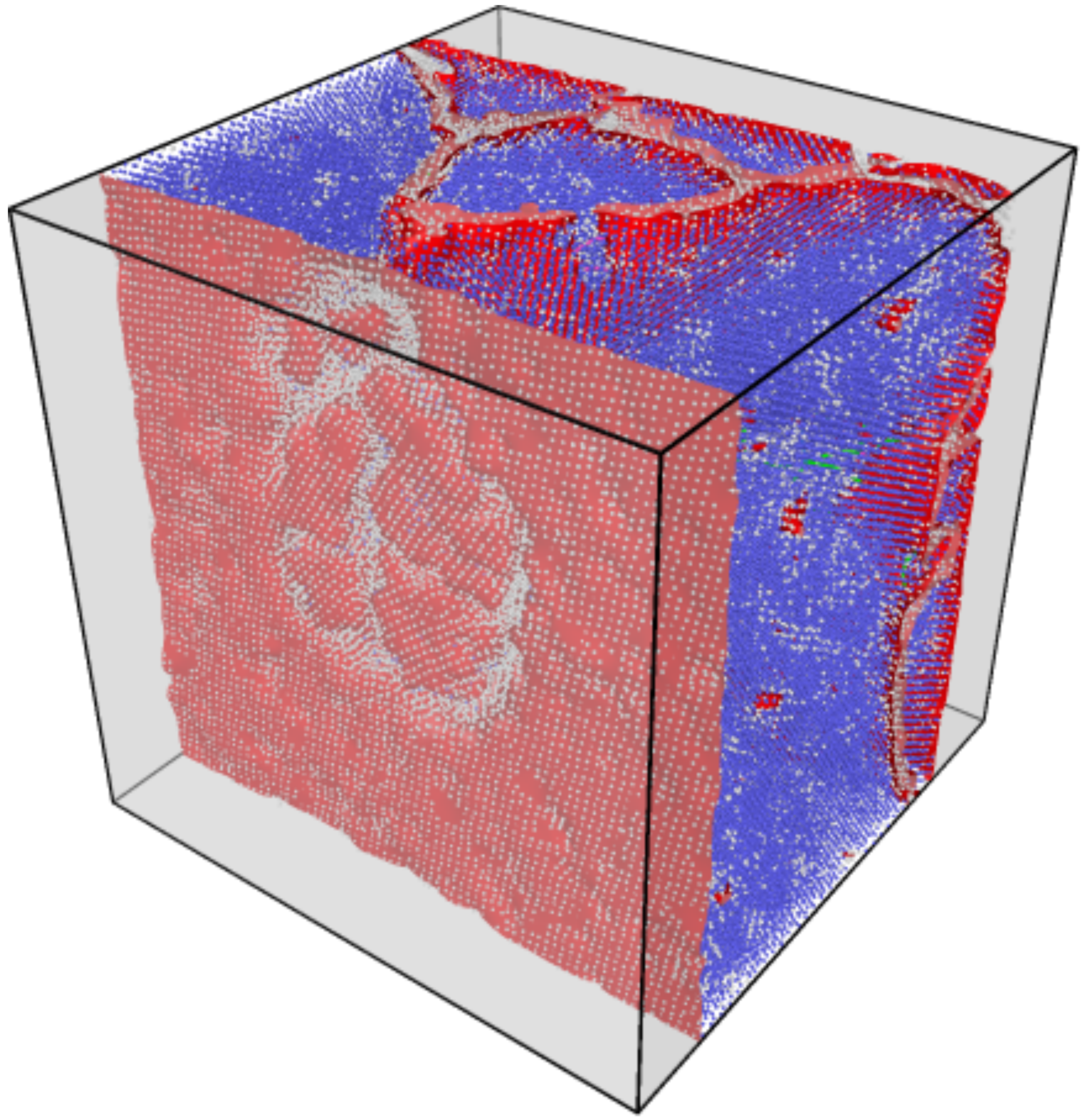
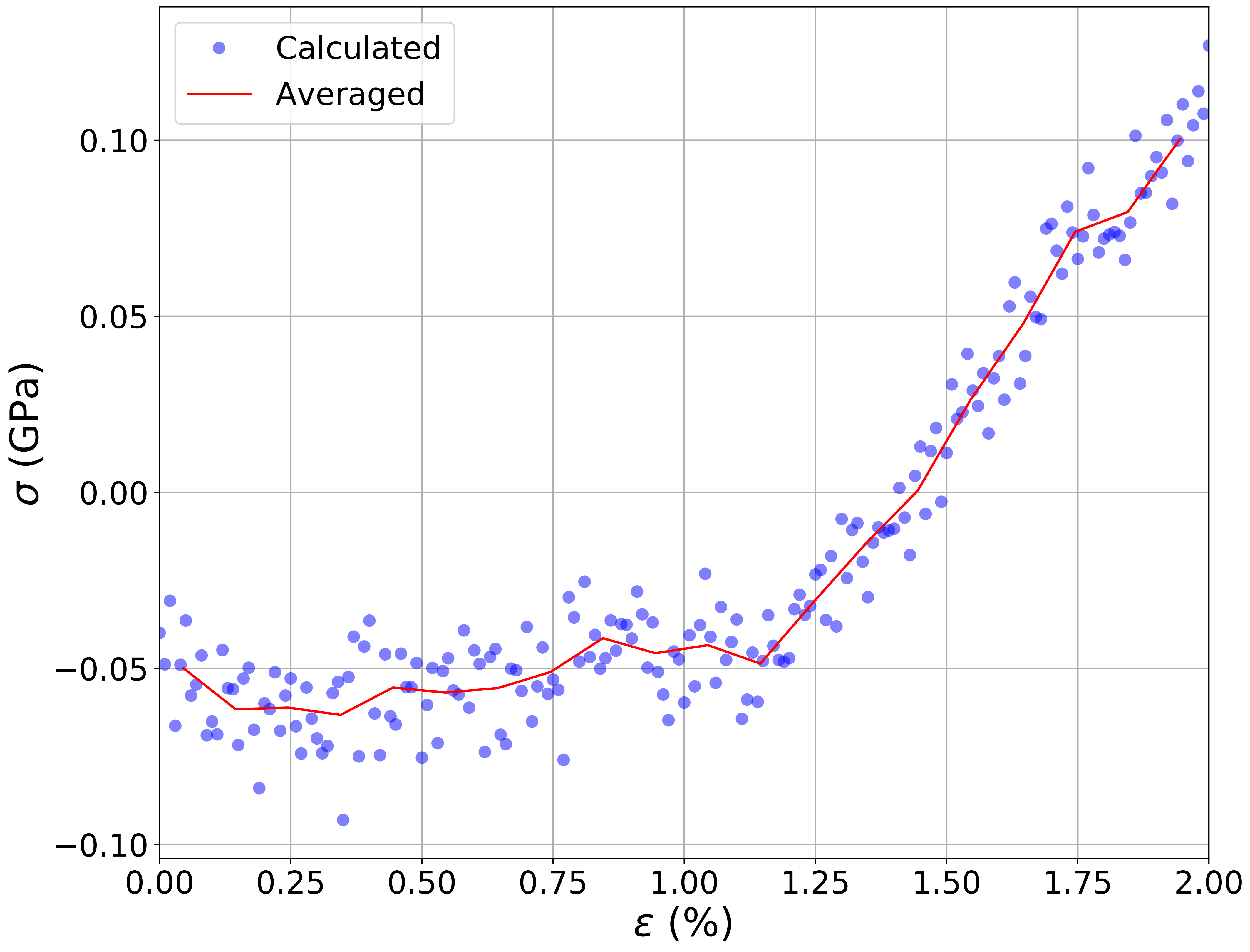
Tensile crystallization



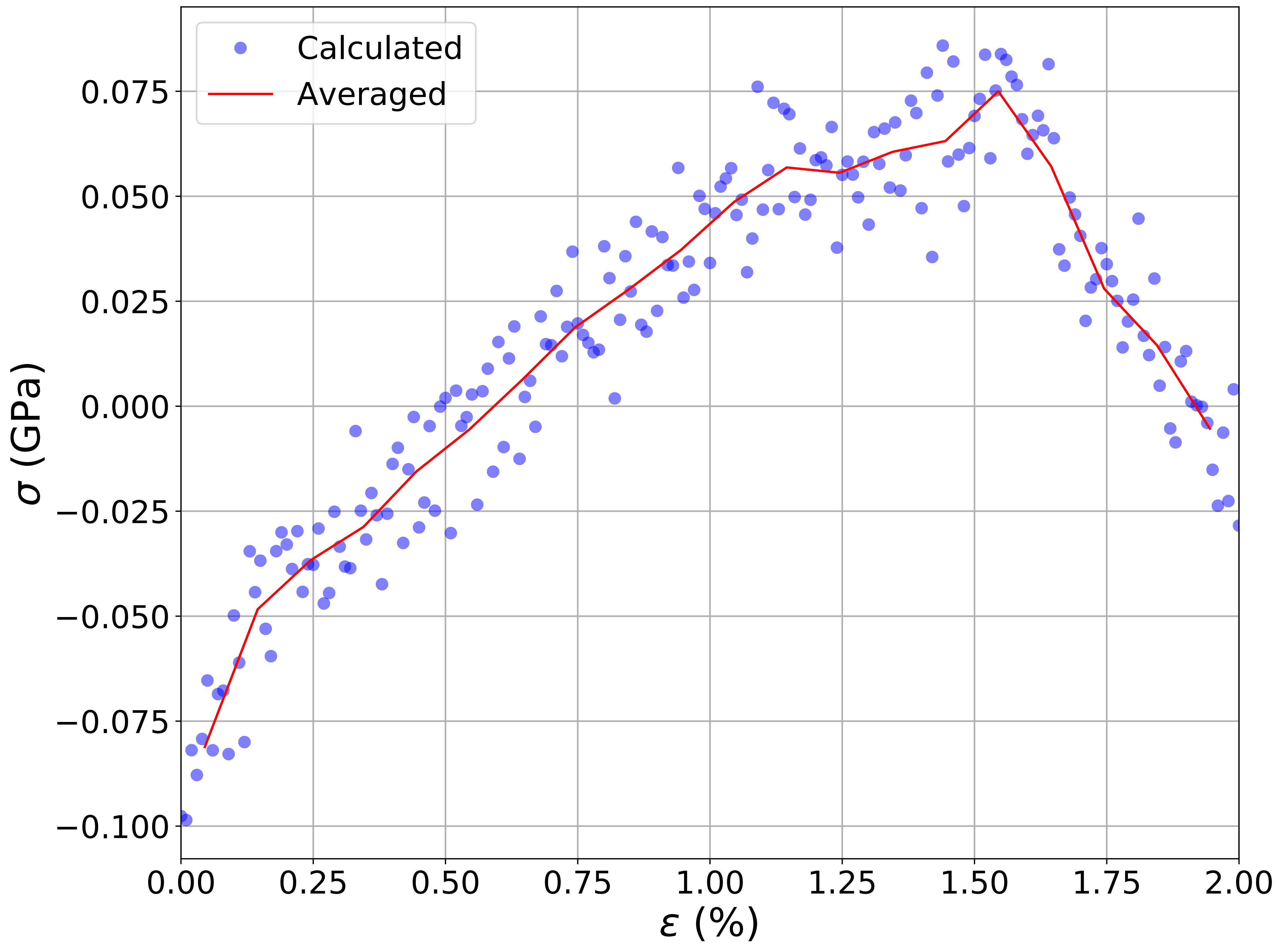
50% Nb
$T \approx 1000$ K



Compression crystallization



25% Nb



75% Nb

$T \approx 1000$ K

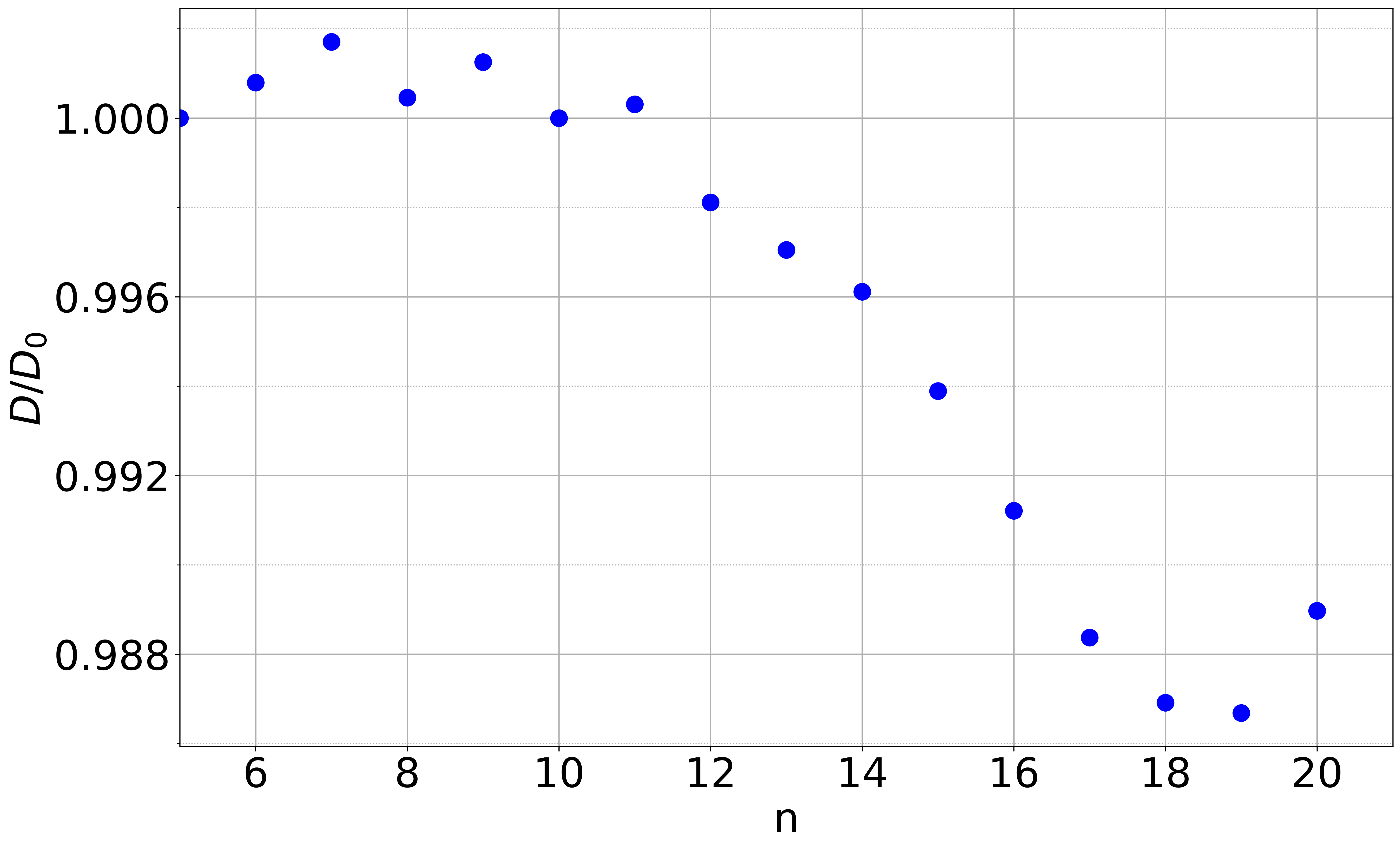
Conclusions

- Glass transition temperature for different concentrations of Nb was determined with the use of the diffusion, viscosity and heat capacity coefficients; the data obtained are in good agreement with each other, with the data determined earlier, as well as with the available experimental data.

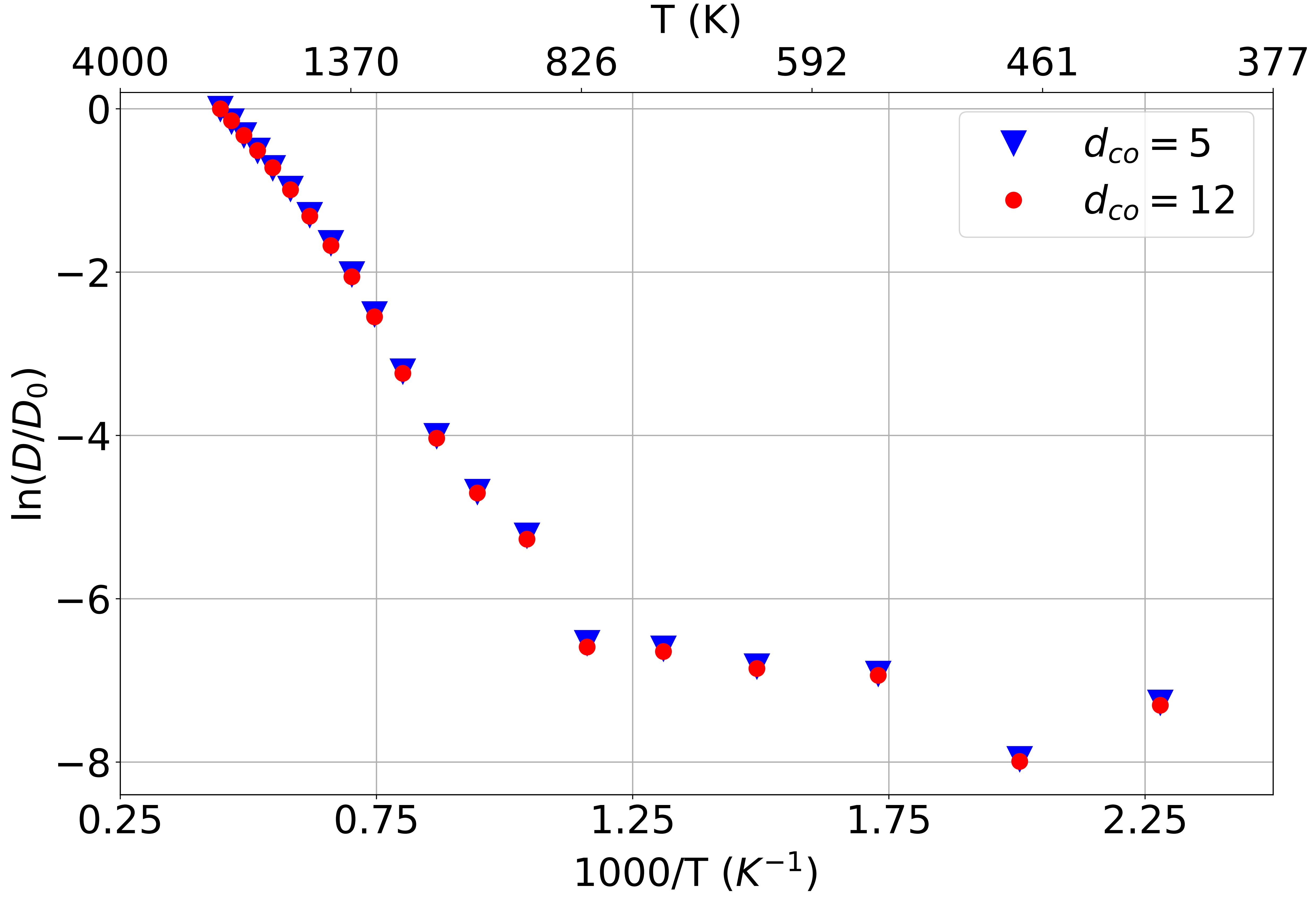
- The dependence of Young's modulus on the percentage of Nb content was explained using the deformation mechanism of amorphous alloys. The hysteresis observed during compression and reverse tension is also explained by the deformation mechanism.

- It is shown that crystallization of the amorphous alloy occurs during high-temperature deformation.

Diffusion coefficient



Diffusion coefficient in a melt with 65 % Nb on the of cut-off periods



Diffusion coefficient on temperature for 65% Nb, cut-off distance 12 and 5 periods

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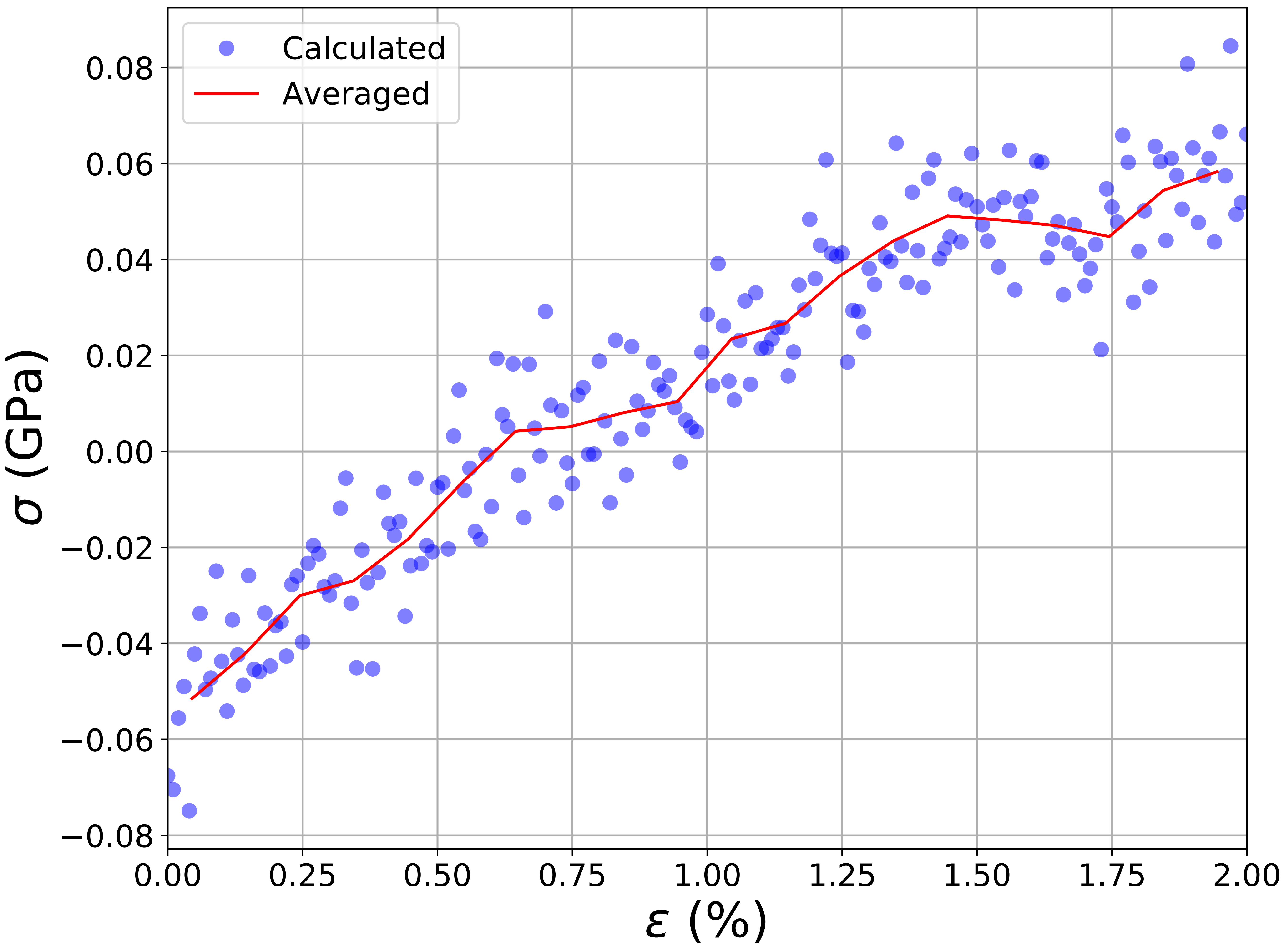
High temperature compression

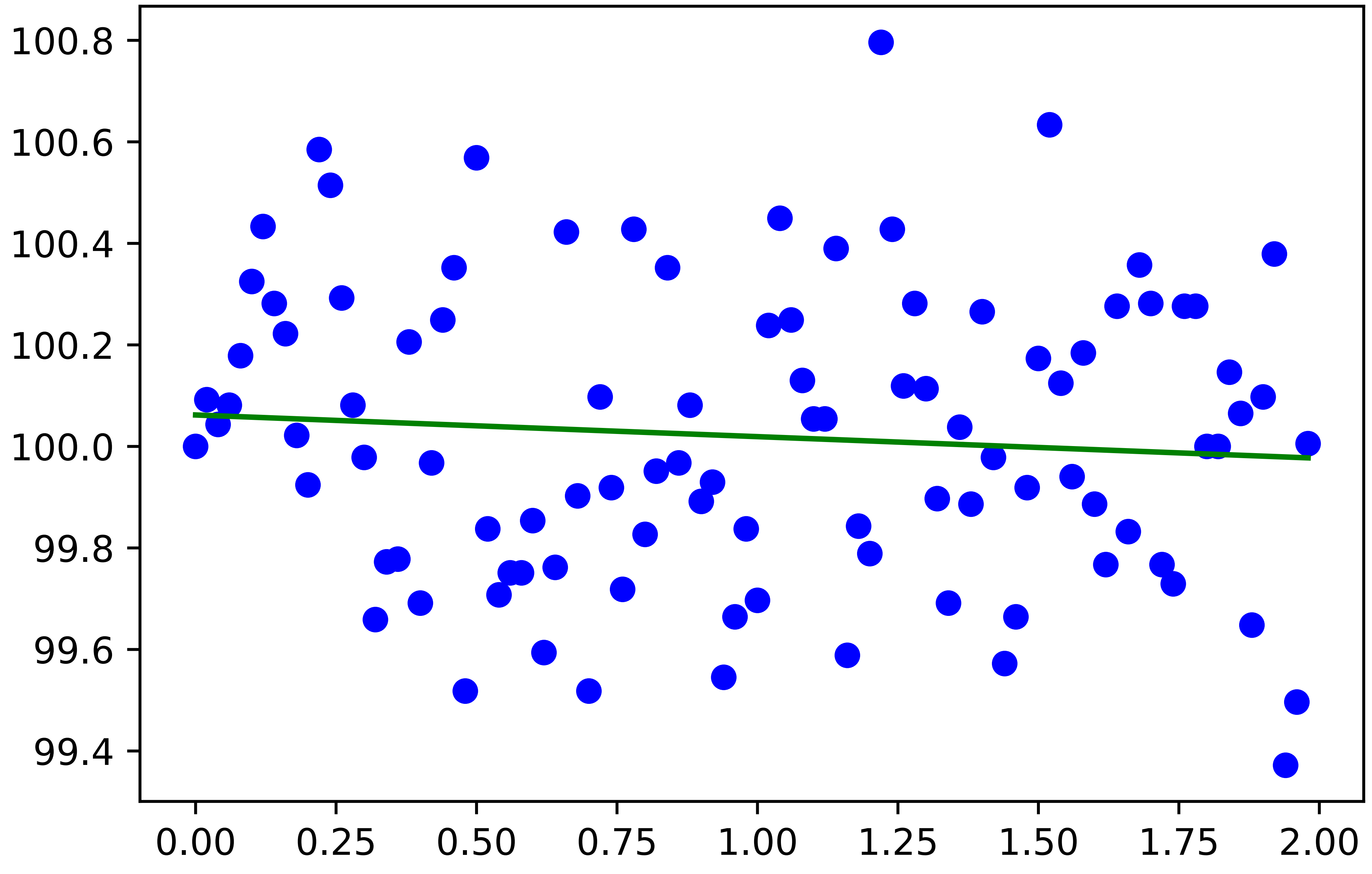


$T \approx 1000$ K

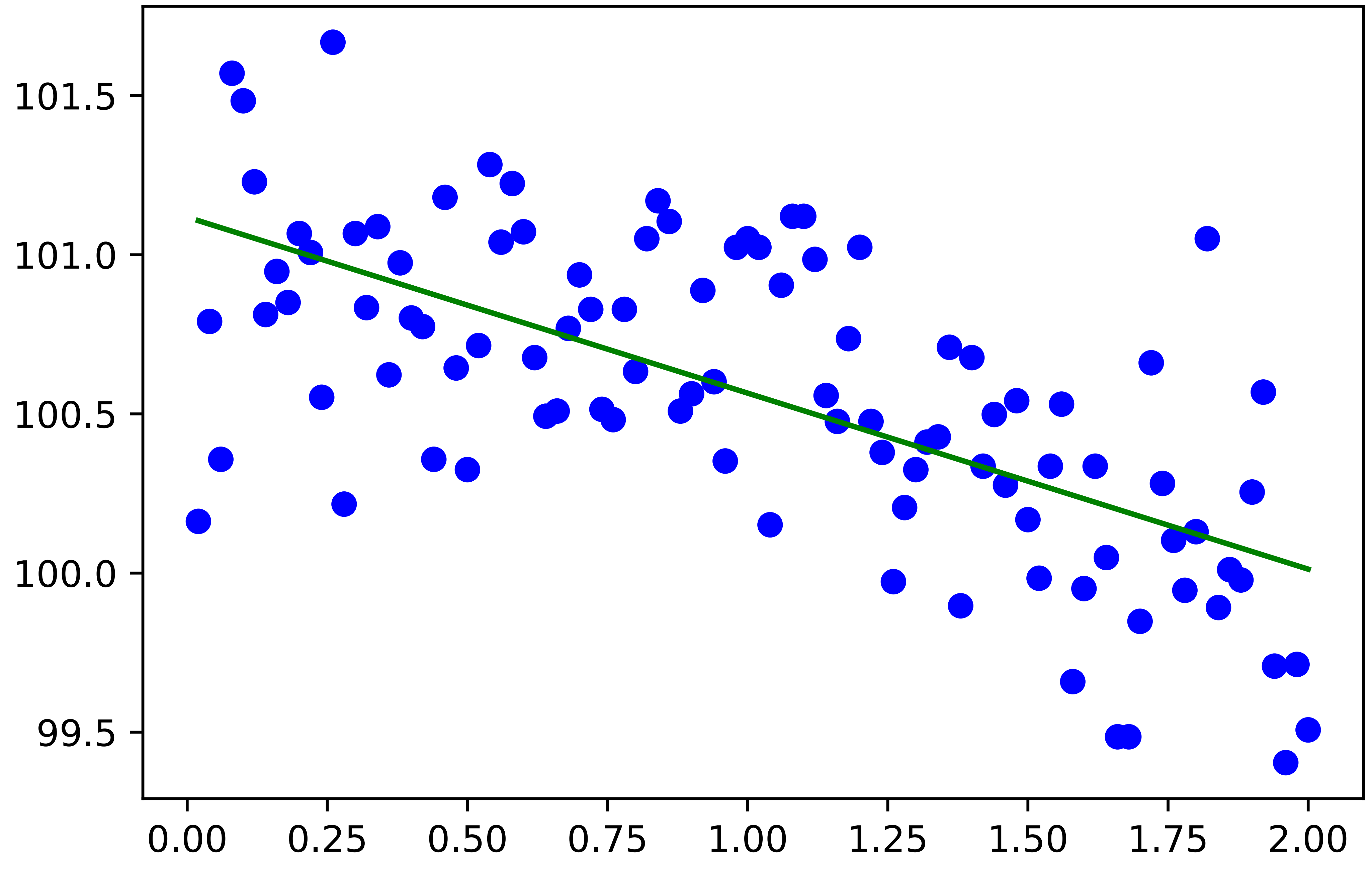
50% Nb

Structure during deformation

50% Nb



compression



tension

Glass transition temperature

%, Nb	$T(K)$ *Heat capacity*, $\Delta T = 30K$	$T(K)$ *Diffusion coefficient*, $\Delta T = 90K$	$T(K)$ *Viscosity coefficient* , $\Delta T = 90$
25	600	750	-
27,5	650	750	-
30	650	725	1000
35	750	800	1050
40	800	800	1000
45	850	900	1100
50	900	900	1000
55	950	900	1000
65	1050	900	-
75	1000	1000	-

Glass transition temperature

	$T(K)$ *Square under second peak,* $\Delta T = 10K$		$T(K)$ *Vendt-Abraham criterium,* $\Delta T = 50K$	$T(K)$ *Icosahedral clusters* $\Delta T = 50K$
%, Nb	cooling	heating	heating	heating
25	1100	1050	1000	1000
27,5	1100	1050	1000	1000
30	1050	1100	1200	1100
35	1000	1100	1150	1150
40	1200	1250	1200	1200
45	1150	1050	1200	1100
50	1100	1050	1200	1200
55	1000	1100	1200	1200
65	1000	1100	1100	1100
75	900	800	1000	1000

Plan

- Research motivation
- Molecular dynamics model
- Glass transition temperature
- Elastic properties
- Conclusions