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## Viscosity of liquid Na-K alloys from molecular dynamics simulations

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## Introduction

The **viscosity** of **liquid metals** and **alloys** is known to be very **low** (lower than water), which leads to several potential applications, like reactor coolant in the case of **Na-K** [1]. However, due to **difficulties** to measure such low viscosity, and because alkalis are highly reactive, there are **no recent experimental data** of the viscosity of this alloy. In that respect, **simulation** seems to be an indispensable way to gain access to these data.

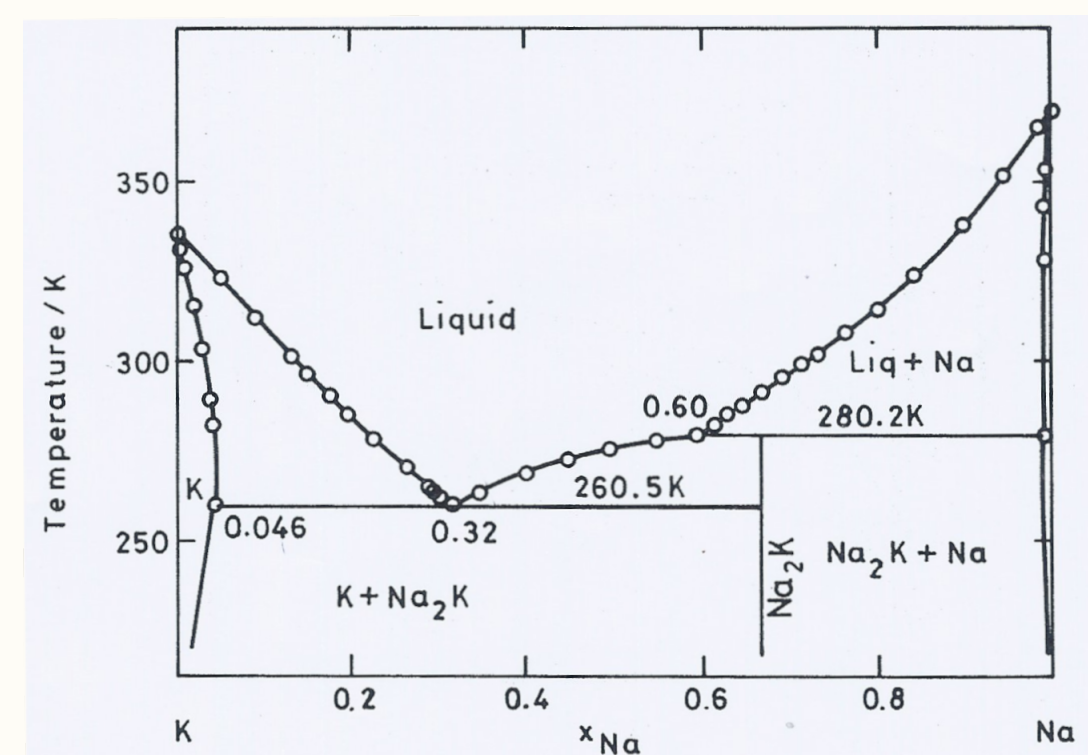
The **composition and temperature dependence** of the **shear viscosity** of **Na-K alloys** is analysed

► Nine compositions at 373 K:

- Na<sub>10</sub>-K<sub>90</sub>
- Na<sub>20</sub>-K<sub>80</sub>
- Na<sub>30</sub>-K<sub>70</sub>
- Na<sub>40</sub>-K<sub>60</sub>
- Na<sub>50</sub>-K<sub>50</sub>
- Na<sub>60</sub>-K<sub>40</sub>
- Na<sub>70</sub>-K<sub>30</sub>
- Na<sub>80</sub>-K<sub>20</sub>
- Na<sub>90</sub>-K<sub>10</sub>

► Three different compositions from 280 K to 1000 K:

- Na<sub>10</sub>-K<sub>90</sub>
- Na<sub>50</sub>-K<sub>50</sub>
- Na<sub>90</sub>-K<sub>10</sub>



Phase diagram of the Na-K system [2]

## Methods

### ► Classical molecular dynamics

- Microcanonical ensemble ( $N, V, E$ )
- $N = 2048$  particles
- $\Delta t \approx 0.1$  fs
- 6 000 000 time steps
- Duration of simulation  $\approx 1$  ns
- Verlet algorithm
- Fiolhais potential [3]

### Calculation of the shear viscosity $\eta$

1. Atomic positions  $\vec{r}_{ij}$ , velocities  $\vec{v}_i$  and forces  $\vec{f}_{ij}$  are computed
2. Off-diagonal stress tensor elements

$$\sigma_{\alpha\beta}(t) = -\frac{1}{V} \left( \sum_{i=1}^N m_i \vec{v}_{i\alpha} \vec{v}_{i\beta} + \sum_{i=1}^{N-1} \sum_{j>1}^N \vec{r}_{ij\alpha} \vec{f}_{ij\beta} \right)$$

3. Autocorrelation  $\rightarrow \langle \sigma_{\alpha\beta}(t_0) \cdot \sigma_{\alpha\beta}(t_0 + t) \rangle$
4. Green-Kubo relation

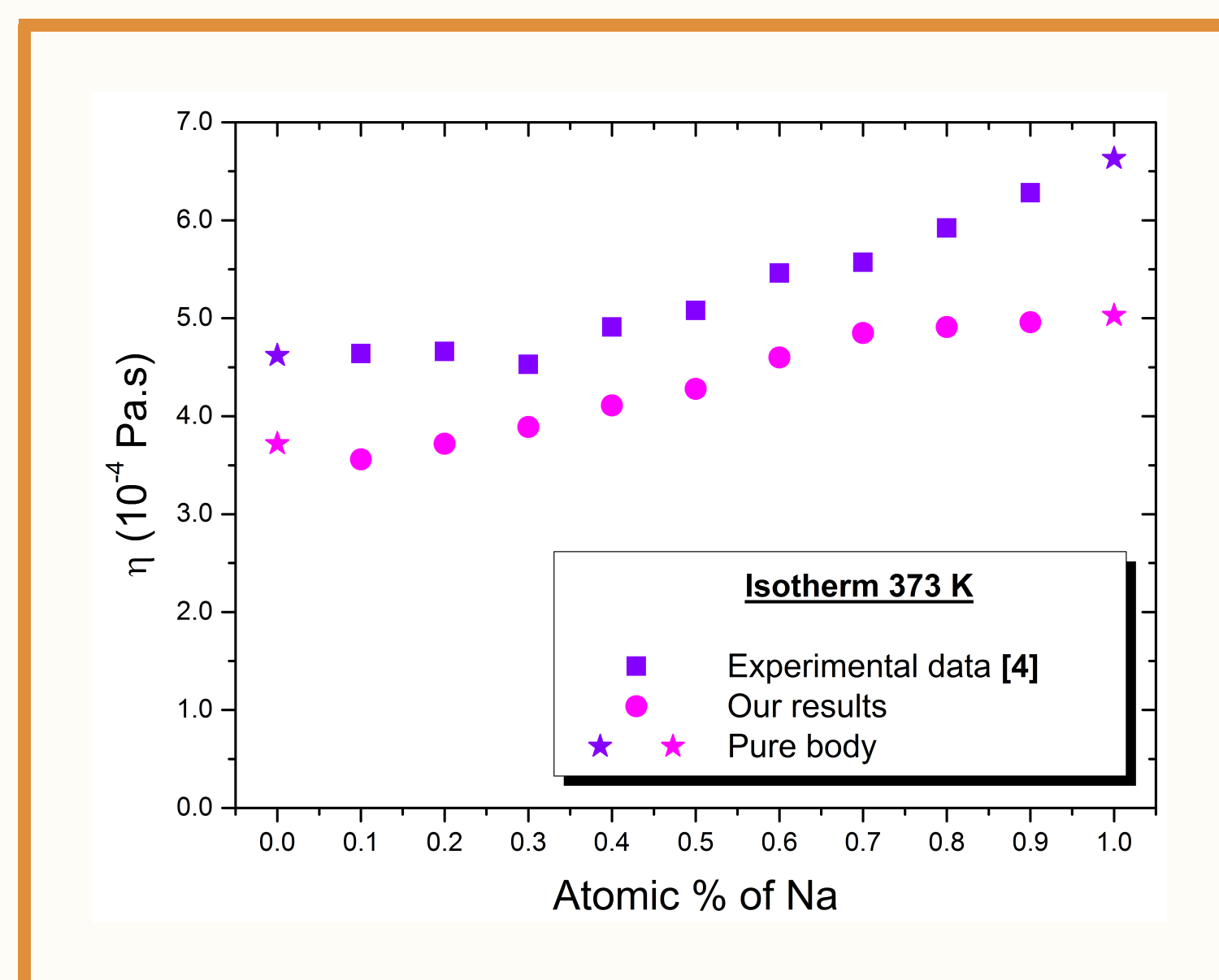
$$\eta_{\alpha\beta} = \frac{V}{k_B T} \int_0^\infty \langle \sigma_{\alpha\beta}(t_0) \sigma_{\alpha\beta}(t_0 + t) \rangle dt$$

### To improve the statistics:

- Average over six stress tensor elements:  $\sigma_{xy}, \sigma_{yz}, \sigma_{xz}, \frac{1}{2}(\sigma_{xx} - \sigma_{yy}), \frac{1}{2}(\sigma_{yy} - \sigma_{zz}), \frac{1}{2}(\sigma_{xx} - \sigma_{zz})$
- Successive shifts of time origin in Green-Kubo relation
- Average over eight different runs

## Results

Statistical error on the simulation results is about 5 %



Viscosity of Na-K alloy vs concentration at 373 K

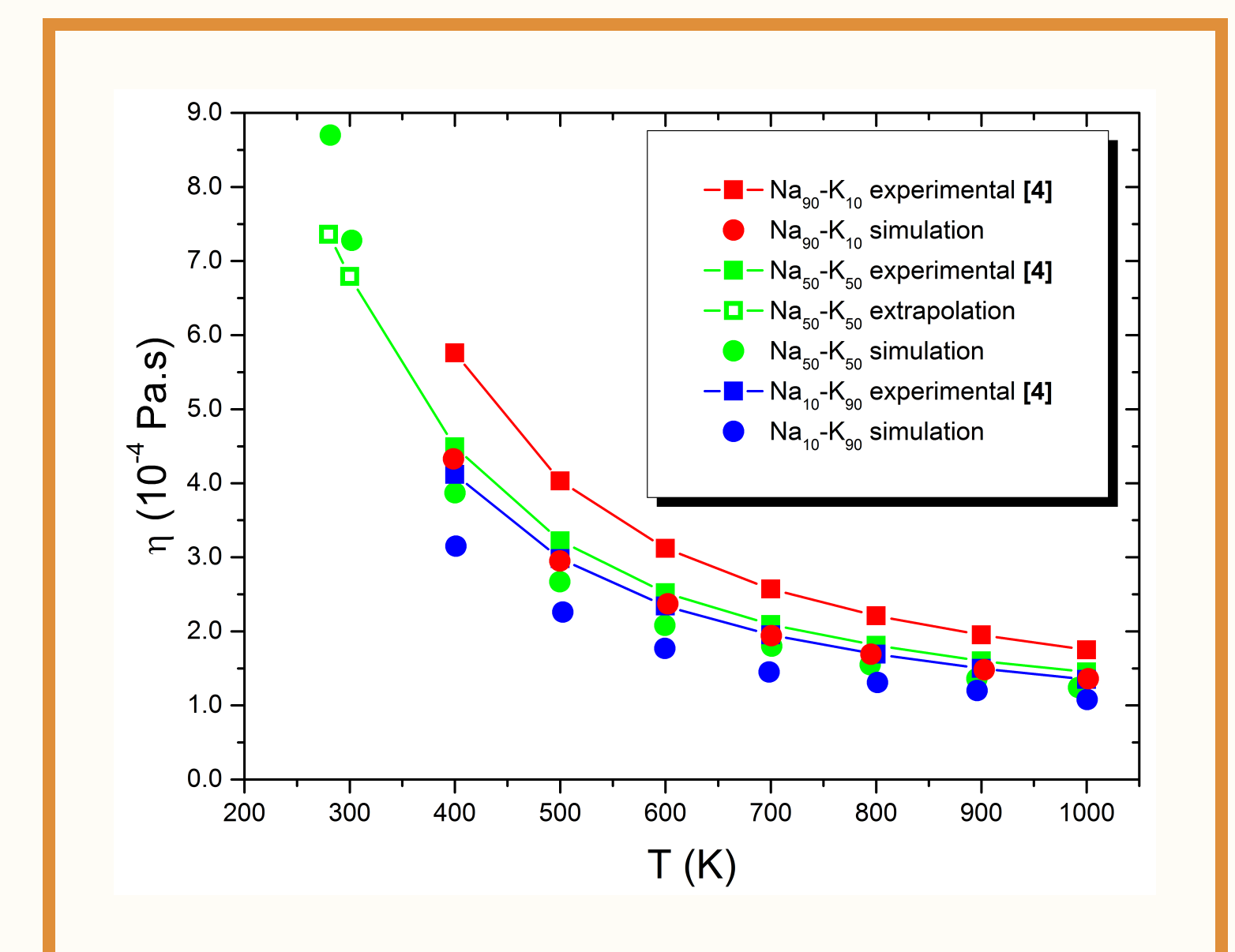
Agreement with experiment [4]

Shift but same trend

- ↔ Inaccuracy of the potential
- ↔ Impurities in the experiments

η increases monotonously with Na concentration

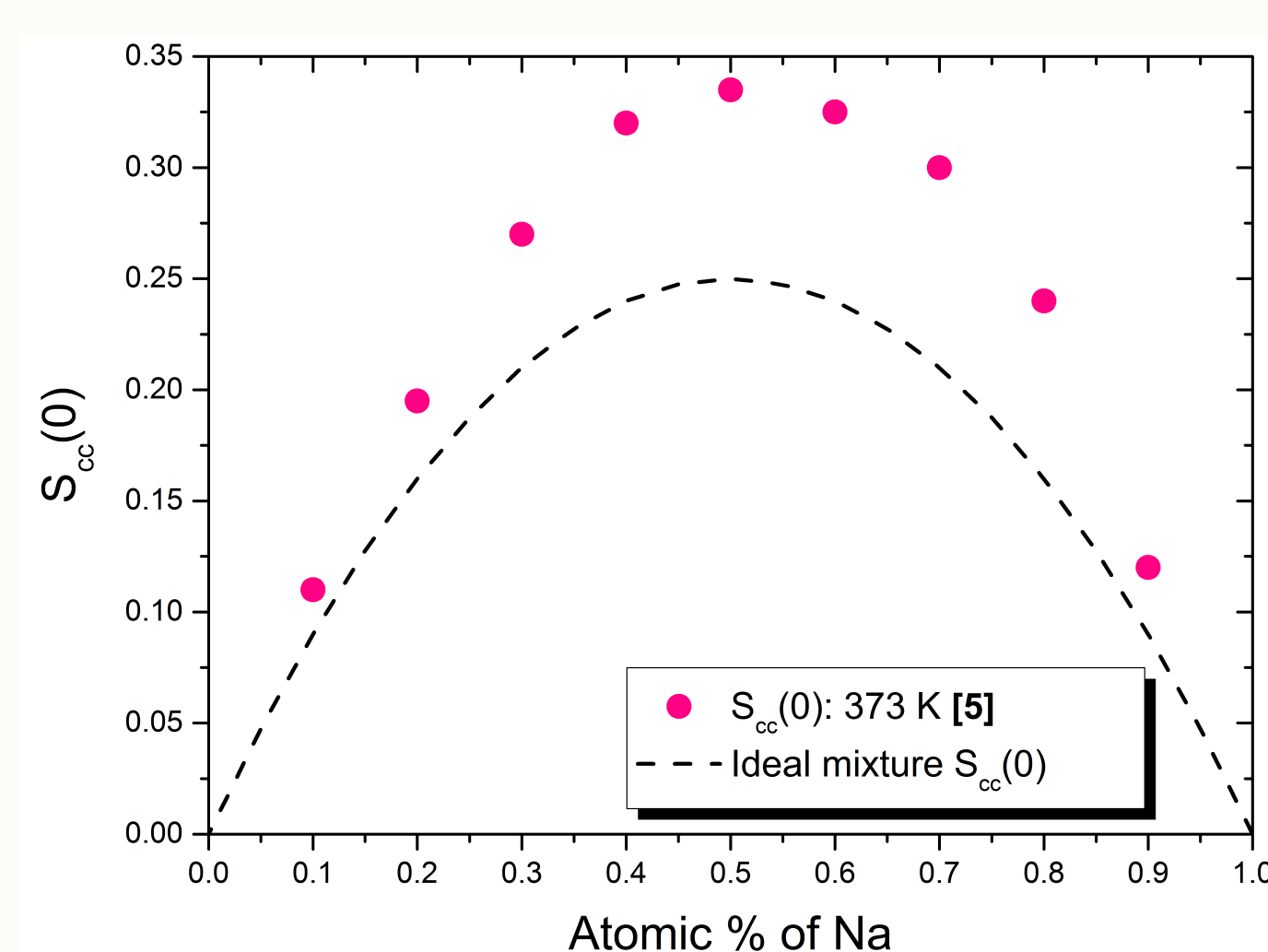
- $T \searrow \Rightarrow \eta \nearrow$
- $Na \searrow \Rightarrow \eta \searrow$



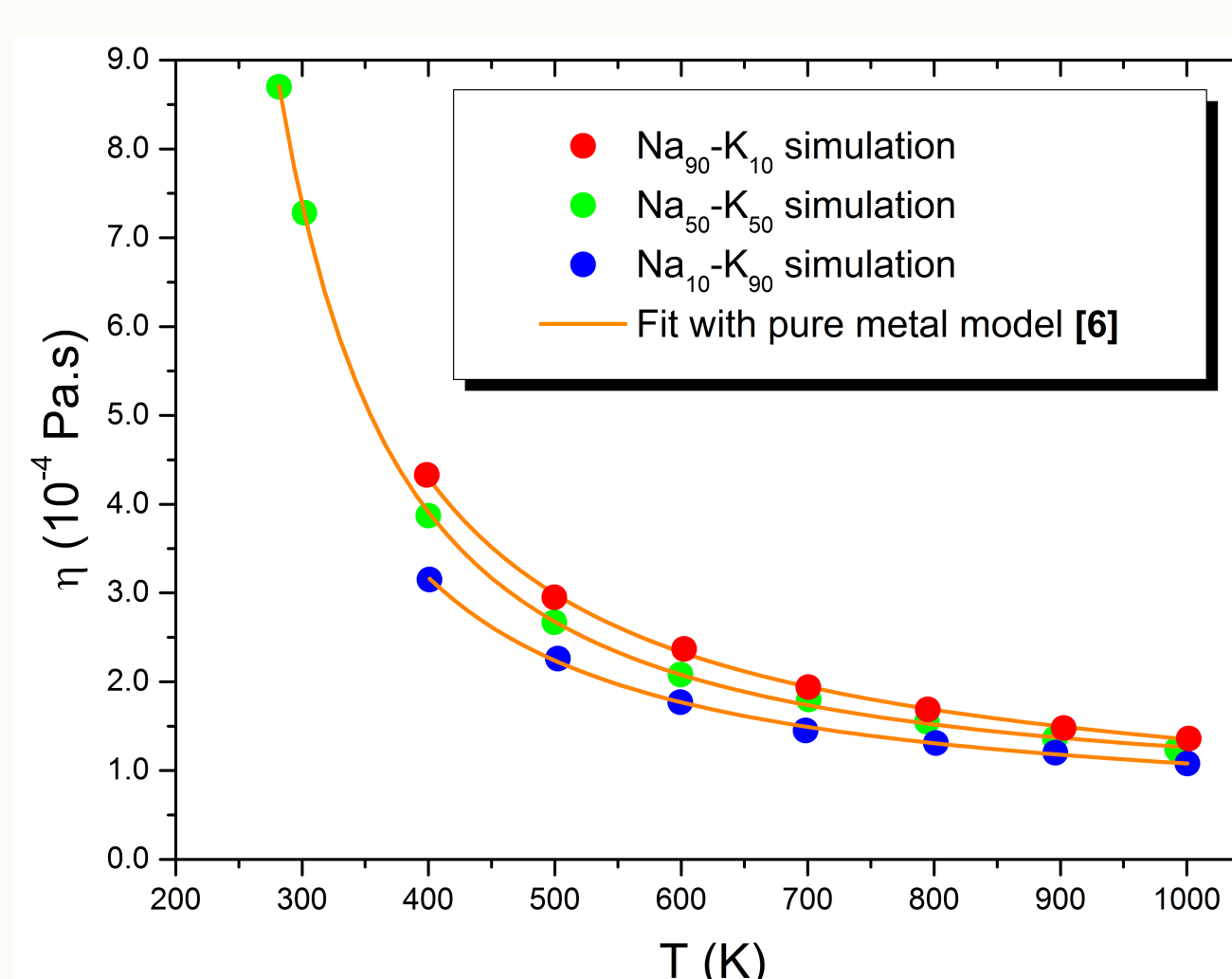
Viscosity of Na-K alloy vs temperature for three studied compositions

Chemical order:

- Bathia-Thornton partial structure factor  $S_{cc}(q=0) > c_{Na}c_K$
- ↓
- Homocoordination tendencies
- **Weak chemical order** [5]



Values of  $S_{cc}(0)$  for Na-K alloy vs composition at 373 K



Simulation data fitted by pure metal model

Fit by equation for pure metal [6]:

$$\eta(T) = (AT^2 + C) e^{B/T}$$

	A (Pa.s.K <sup>-2</sup> )	B (K)	C (Pa.s)
Na <sub>90</sub> -K <sub>10</sub>	$-7.94 \times 10^{-12}$	706.11	$7.00 \times 10^{-5}$
Na <sub>50</sub> -K <sub>50</sub>	$9.03 \times 10^{-13}$	762.75	$6.00 \times 10^{-5}$
Na <sub>10</sub> -K <sub>90</sub>	$-2.94 \times 10^{-12}$	688.75	$6.00 \times 10^{-5}$

## Conclusion

Simulation and experimental data follow the **same trend**. In qualitative terms, the **Fiolhais potential** seems to be **successful** to compute the **shear viscosity** of **Na-K**.

As a **consequence of the weak chemical order** of the alloy:

- The evolution of the **viscosity of Na-K versus concentration** is **rather smooth**.
- The evolution of the **viscosity of Na-K versus temperature** is similar to that of a **pure one component fluid**. The **shear viscosity** can then be calculated by the **relation** proposed by Meyer *et al.* for **liquid Na** [6].

## References

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