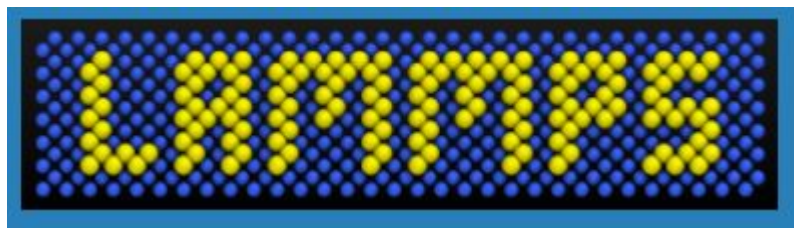


Počítačové simulace pevných látek

Radim Novák

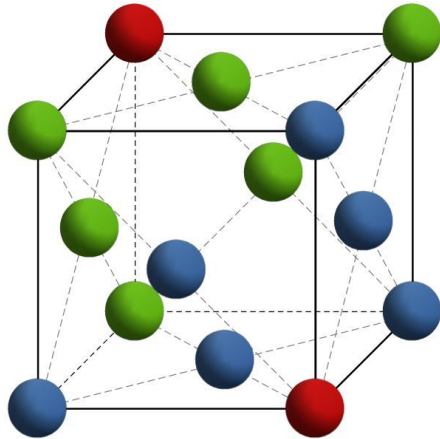
LAMMPS, OVITO

- klasický MD software
- vizualizační software

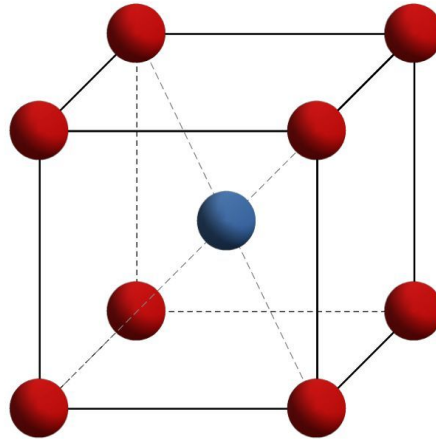


Krystalová mřížka

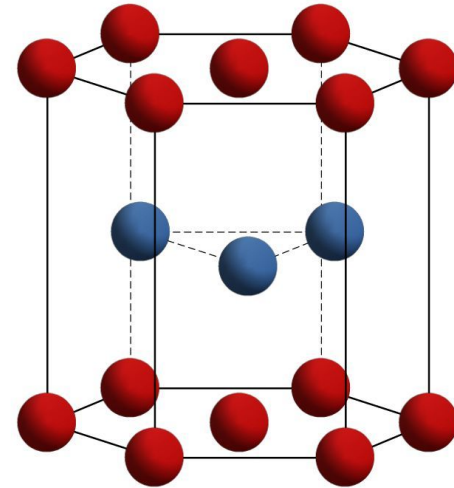
decreasing ductility



fcc

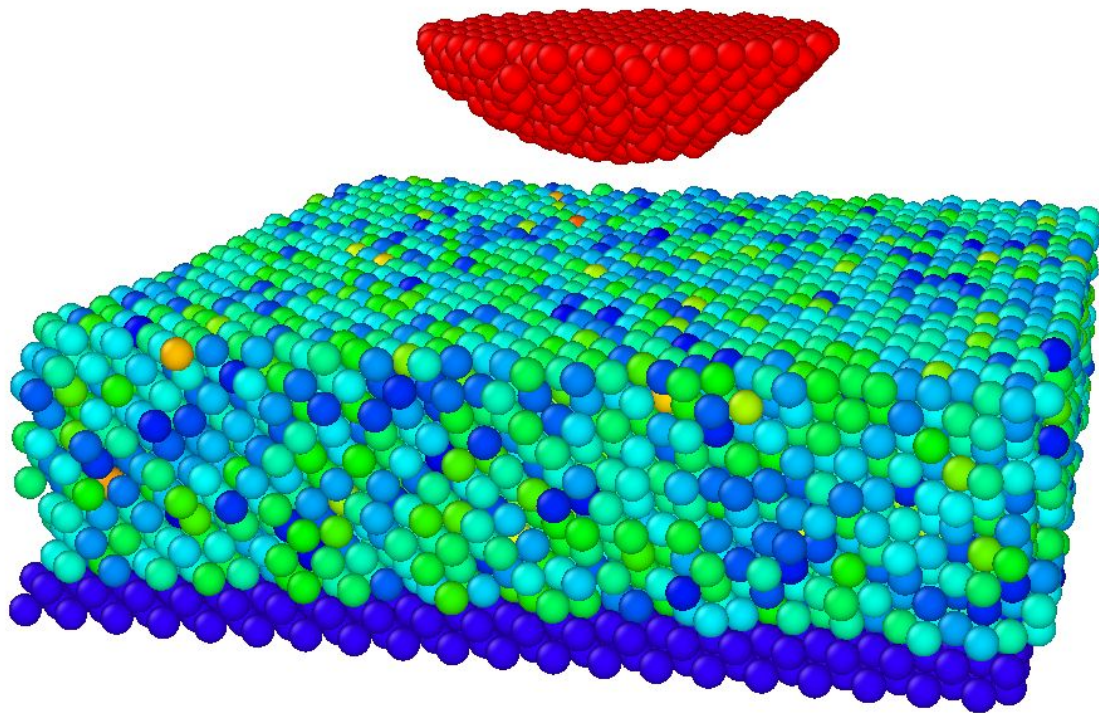


bcc



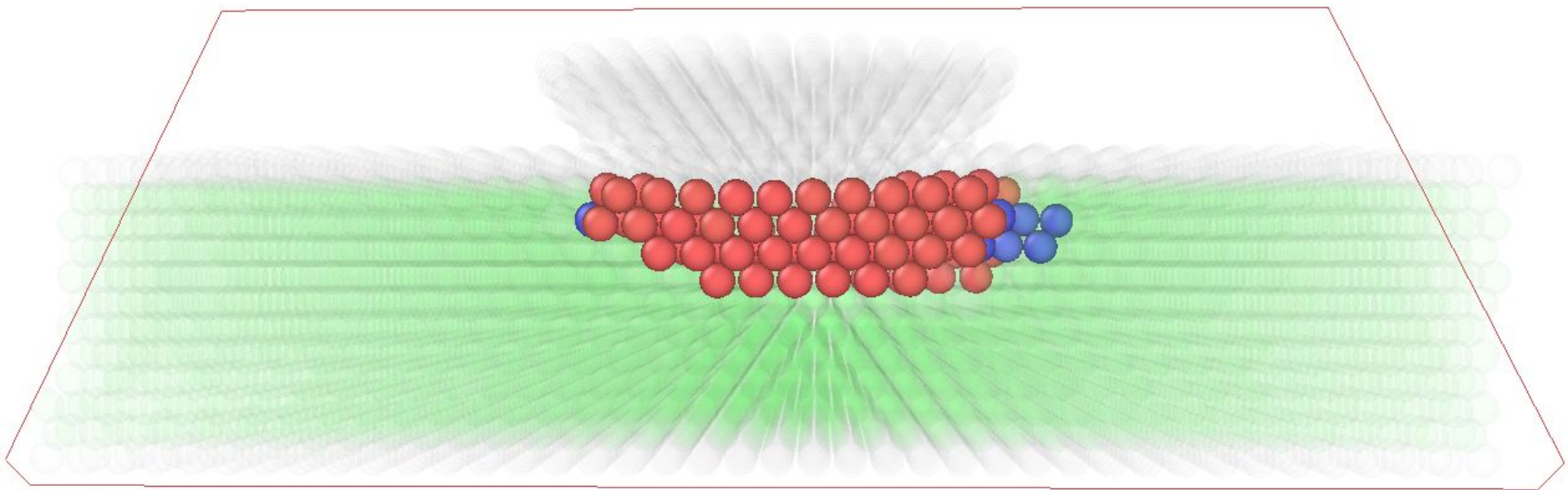
hcp

Simulace

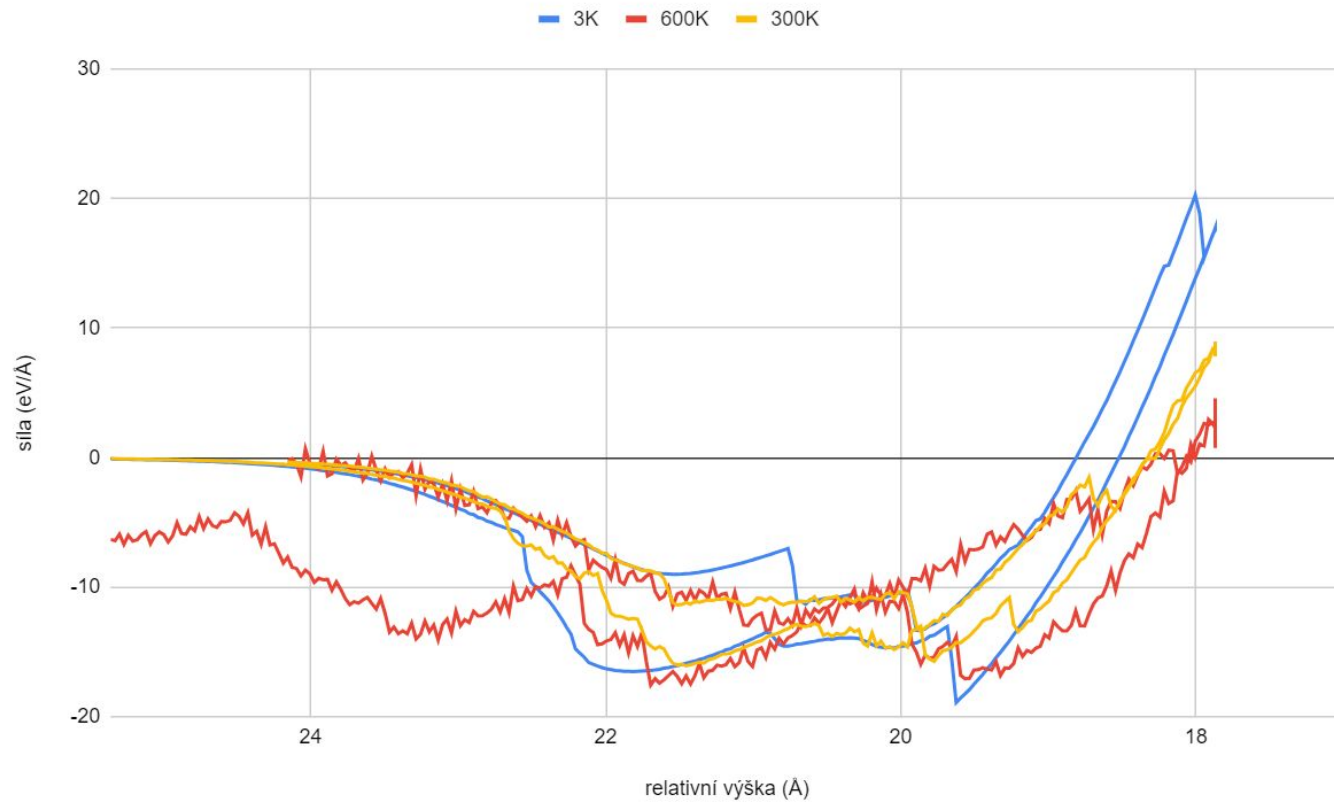


EAM

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

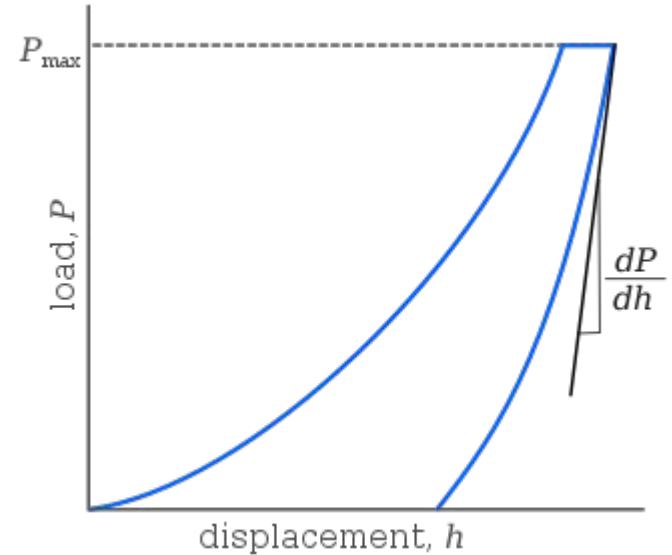


Výsledky simulace



redukovaný Youngův modul pružnosti

$$E_r = \frac{1}{\beta} \frac{\sqrt{\pi}}{2} \frac{S}{\sqrt{A_p(h_c)}}$$



Spočtené moduly

.	3K	300K	600k
E_r [GPa]	236	161	152

Možnost dalšího výzkumu

Poděkování

Chtěl bych tímto poděkovat mému garantovi panu Janu Drahokoupilovi a panu Miroslavu Lebedovi.

