

Modeling of alloys: Determining the elastic properties of single grains in the ultrafine-grained W-Cr composite

Andrzej P. Kądzielawa

andrzej.piotr.kadzielawa@vsb.cz



IT4INNOVATIONS
NÁRODNÍ SUPERPOČÍTAČOVÉ
CENTRUM



GRANTOVÁ AGENTURA ČESKÉ REPUBLIKY

within the GAČR project GA20-18392S: *Tailoring thermal stability of W-Cr based alloys for fusion application*

Authors

Jakub Veverka^{a,b}, František Lukáč^{a,c}, Andrzej P. Kądzielawa^{d,e},
Martin Koller^f, Zdeněk Chlup^g, Hynek Hadraba^g, Miroslav Karlík^{b,c},
Dominik Legut^d, Jiřina Vontorová^h, Tomáš Chráska^a, Monika Vilémová^a

^a Institute of Plasma Physics, The Czech Academy of Sciences, Czechia

^b Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czechia

^c Faculty of Mathematics and Physics, Charles University, Czechia

^d IT4Innovations, VŠB - Technical University of Ostrava, Czechia

^e Institute of Theoretical Physics, Jagiellonian University, Poland

^f Institute of Thermomechanics, The Czech Academy of Sciences, Czechia

^g Institute of Physics of Materials, The Czech Academy of Sciences, Czechia

^h Faculty of Materials Science and Technology, VŠB - Technical University of Ostrava, Czechia



ÚSTAV FYZIKY PLAZMATU AV ČR
INSTITUTE OF PLASMA PHYSICS OF THE CAS



UNIVERZITA KARLOVA
Matematicko-fyzikální
fakulta



IT4INNOVATIONS
NÁRODNÍ SUPERPOČÍTAČOVÉ
CENTRUM



UNIWERSYTET
JAGIELŁOŃSKI
W KRAKOWIE



FAKULTA
MATERIÁLOVÉ
TECHNOLOGICKÁ

KATEDRA
CHEMIE

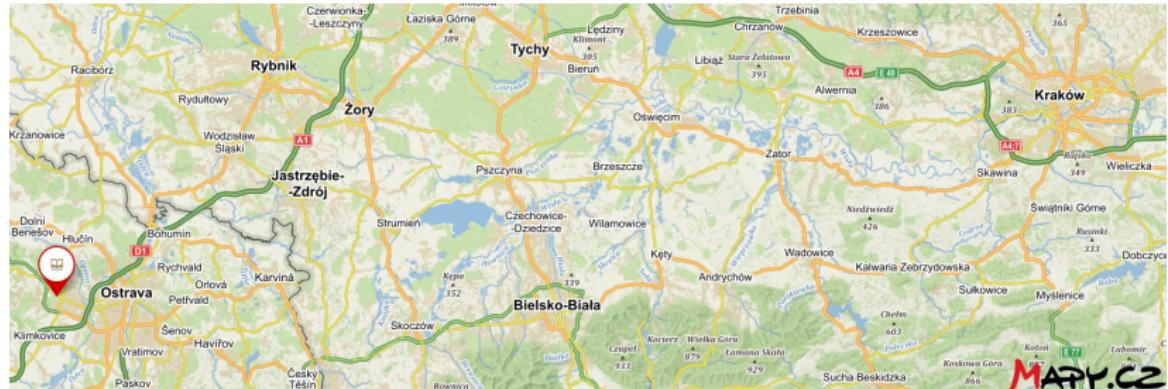


ÚSTAV TERMOMECHANIKY AV ČR, v. v. i.



ÚSTAV FYZIKY MATERIÁLŮ
Akademie věd České republiky, v. v. i.

IT4Innovations národní superpočítacové centrum, Vysoká Škola Báňská-technická Univerzita Ostrava



Andrzej P. Kądzielawa

Modeling of alloys

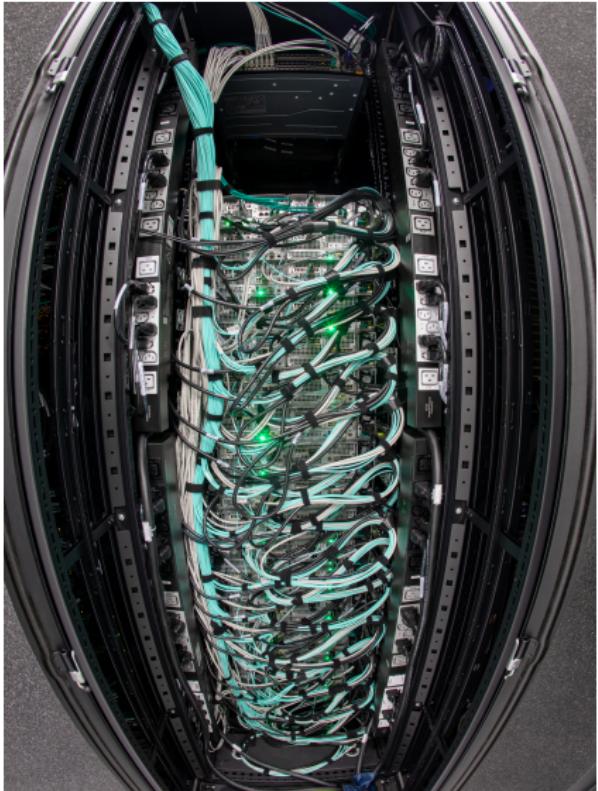


June 25, 2025

Karolina - fastest computational cluster in Czechia

8 71

Karolina, GPU partition - Apollo 6500,
AMD EPYC 7763 64C 2.45GHz, NVIDIA A100
SXM4 40 GB, Infiniband HDR200, HPE
IT4Innovations National Supercomputing
Center, VSB-Technical University of
Ostrava
Czechia



1 Introduction

- Fusion reactors

2 Statistical Mechanics vs Quantum Mechanics

- Enthalpy of formation
- Entropy
- Phonons

3 Special Quasirandom Structures

- Genetic algorithm
- Correlation function

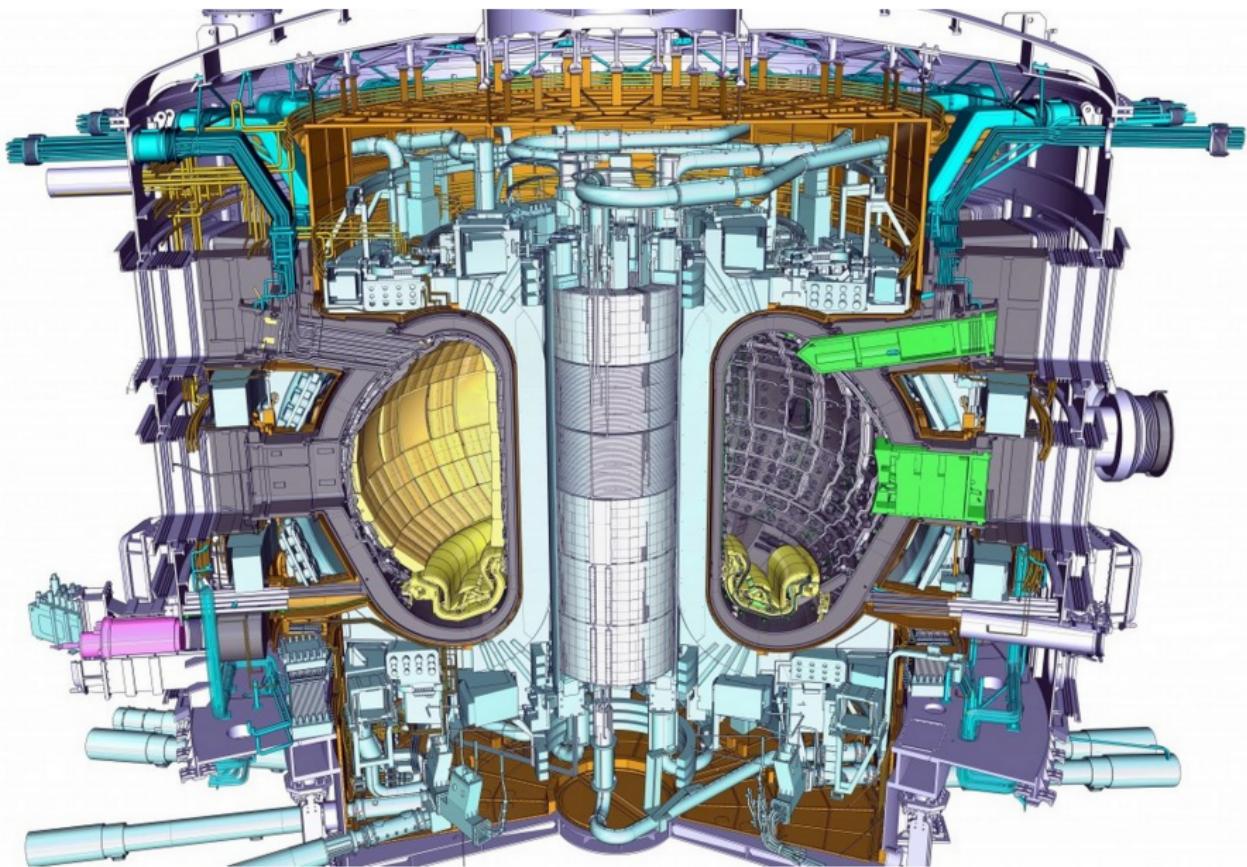
4 Results

- Quasiharmonic approxiamtion
- Energetics

5 Elastic properties

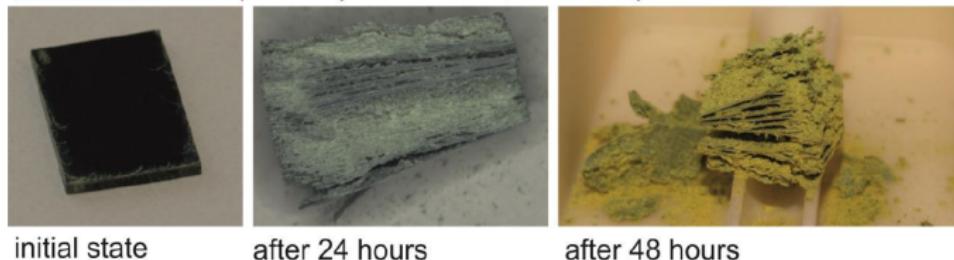
- Special Quasirandom Structures vs Experiment
- Experimental Elastic Moduli

Reactor



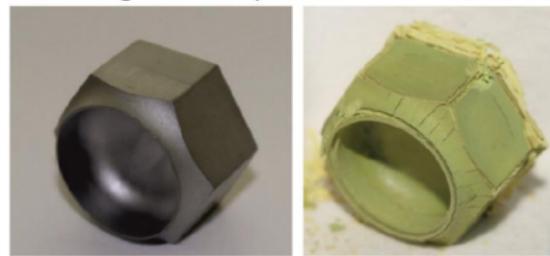
Choice: Tungsten; Problem: Oxidation

Reference: rolled pure W plate: 600 °C, air atmosphere



initial state after 24 hours after 48 hours

Pure tungsten PIM part „tile“: 700 °C, air atmosphere

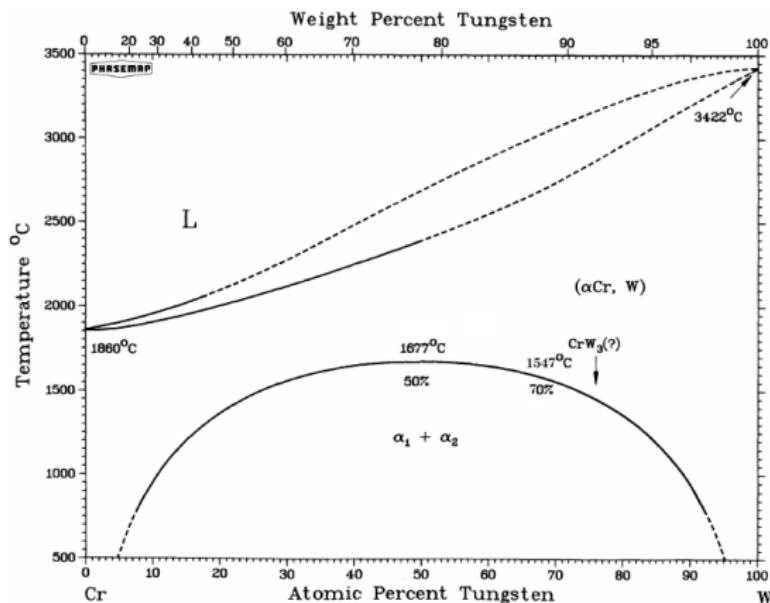


initial state after 4 days

Fig. 17: Oxidation tests on pure tungsten.

S. Antusch, et al., Nucl. Mater. Energy 3-4, 22 (2015).

Tailoring thermal stability of W-Cr based alloys for fusion application (GA20-18392S)



S. V. Nagender Naidu, A. M. Sriramamurthy, and P. Rama Rao, Bull. Alloy Phase Diagr. 5, 289 (1984).

New goal:

To find a more stable $W_xCr_{1-x-\delta}X_\delta$ ($\delta \ll x$). And now this...

Andrzej P. Kądzielawa



VŠB TECHNICKÁ
UNIVERZITA
OSTRAVA

IT4INNOVATIONS
NÁRODNÍ SUPERPOČÍTAČOVÉ
CENTRUM

Monika Vilemová

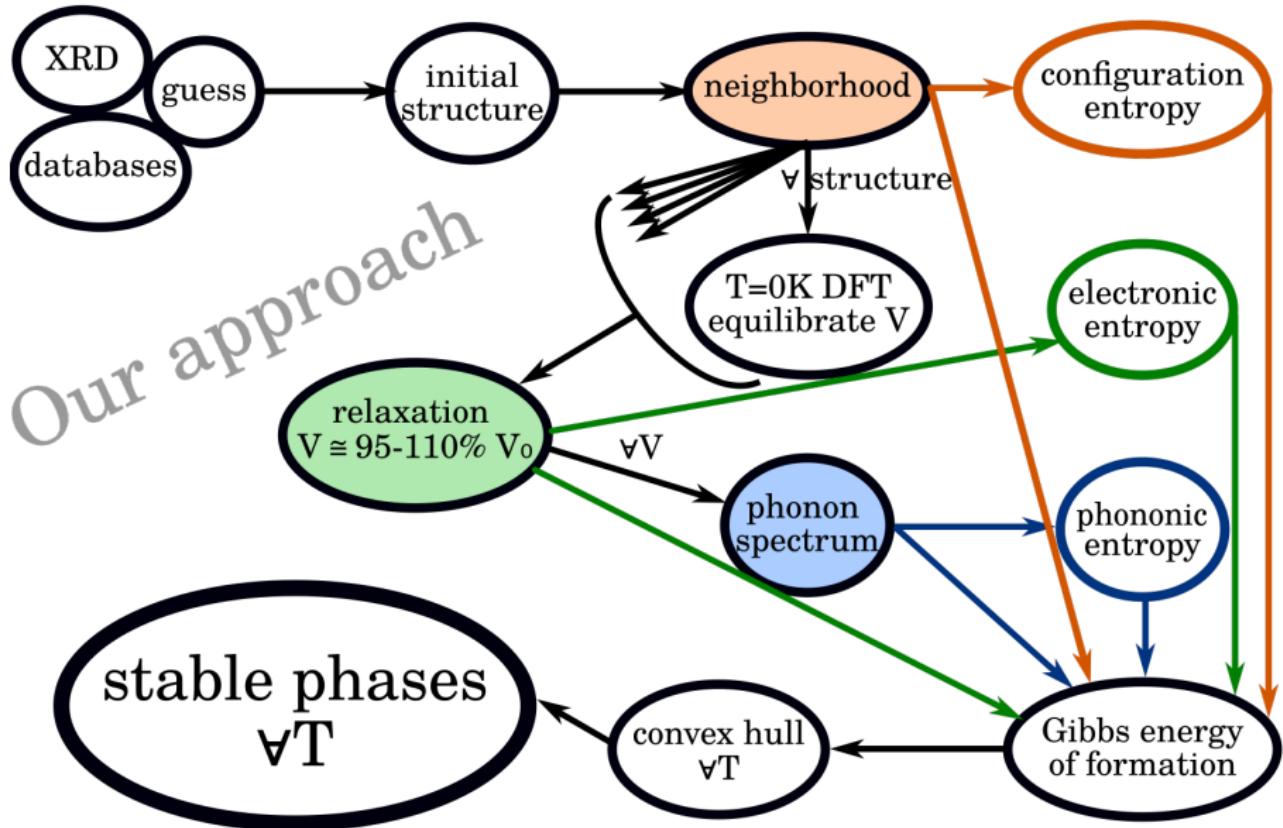


 IPP ÚSTAV FYZIKY PLAZMATU AV ČR
INSTITUTE OF PLASMA PHYSICS OF THE CAS

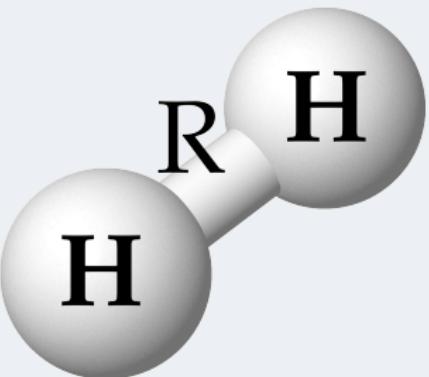
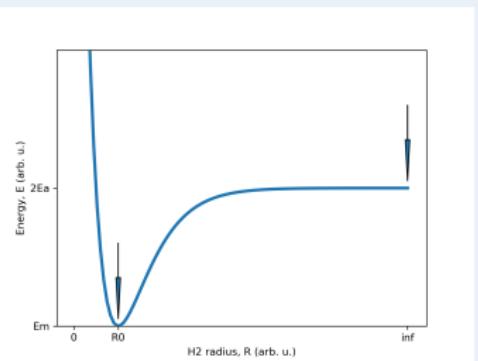
Materials

no-go ($>10^{-1}$ Sv/h)		recycling limit ($<10^{-1}$ Sv/h)		hands-on limit ($<10^{-4}$ Sv/h)			
Eu	$7.15 \cdot 10^{02}$	Cd	$3.69 \cdot 10^{-02}$	Lu	$8.37 \cdot 10^{-05}$	Fe	$4.25 \cdot 10^{-06}$
Tb	$2.30 \cdot 10^{02}$	Os	$3.65 \cdot 10^{-02}$	Ce	$6.84 \cdot 10^{-05}$	Au	$2.43 \cdot 10^{-06}$
Ho	$5.56 \cdot 10^{01}$	Tm	$3.31 \cdot 10^{-02}$	Re	$6.01 \cdot 10^{-05}$	P	$8.67 \cdot 10^{-07}$
Ag	$2.90 \cdot 10^{01}$	Al	$2.88 \cdot 10^{-02}$	Ta	$5.07 \cdot 10^{-05}$	Ar	$6.28 \cdot 10^{-07}$
Nb	$1.12 \cdot 10^{01}$	Ni	$1.14 \cdot 10^{-02}$	Ca	$2.83 \cdot 10^{-05}$	Y	$2.45 \cdot 10^{-07}$
Bi	$5.39 \cdot 10^{00}$	Cu	$1.10 \cdot 10^{-02}$	Pb	$2.60 \cdot 10^{-05}$	Mg	$6.39 \cdot 10^{-08}$
Ir	$4.57 \cdot 10^{00}$	Kr	$9.83 \cdot 10^{-03}$	Br	$2.51 \cdot 10^{-05}$	Tl	$4.90 \cdot 10^{-08}$
Sm	$2.89 \cdot 10^{00}$	Cs	$6.29 \cdot 10^{-03}$	Zn	$2.12 \cdot 10^{-05}$	Mg	$1.37 \cdot 10^{-08}$
Co	$1.62 \cdot 10^{00}$	Sn	$2.35 \cdot 10^{-03}$	Pr	$1.69 \cdot 10^{-07}$	Se	$5.96 \cdot 10^{-09}$
Dy	$7.96 \cdot 10^{-01}$	Rb	$1.80 \cdot 10^{-03}$	W	$1.54 \cdot 10^{-05}$	V	$4.32 \cdot 10^{-09}$
Gd	$6.79 \cdot 10^{-01}$	Nd	$1.63 \cdot 10^{-03}$	Yb	$1.42 \cdot 10^{-05}$	S	$3.02 \cdot 10^{-09}$
Xe	$5.55 \cdot 10^{-01}$	Sc	$5.70 \cdot 10^{-04}$	K	$8.60 \cdot 10^{-06}$	I	$9.59 \cdot 10^{-10}$
Hf	$3.81 \cdot 10^{-01}$	Ru	$3.66 \cdot 10^{-04}$	Hg	$7.20 \cdot 10^{-06}$	Na	$1.56 \cdot 10^{-10}$
Er	$3.78 \cdot 10^{-01}$	La	$3.24 \cdot 10^{-04}$	In	$6.84 \cdot 10^{-06}$	Cr	$3.11 \cdot 10^{-11}$
Pt	$3.29 \cdot 10^{-01}$	Sb	$3.16 \cdot 10^{-04}$	Te	$6.84 \cdot 10^{-06}$	Ga	$1.78 \cdot 10^{-11}$
Ba	$2.44 \cdot 10^{-01}$	Zr	$2.97 \cdot 10^{-04}$	Si	$6.71 \cdot 10^{-06}$	Ge	$7.04 \cdot 10^{-12}$
Pd	$1.86 \cdot 10^{-01}$	Ti	$1.20 \cdot 10^{-04}$	Rh	$4.55 \cdot 10^{-06}$	As	$1.15 \cdot 10^{-18}$
Mo	$1.64 \cdot 10^{-01}$	Sr	$1.07 \cdot 10^{-04}$	Cl	$4.54 \cdot 10^{-06}$		

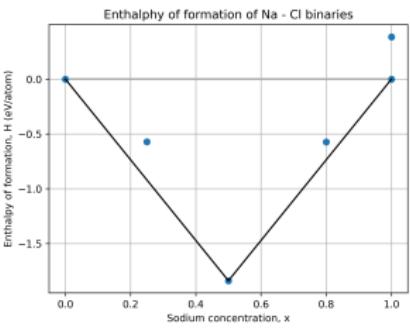
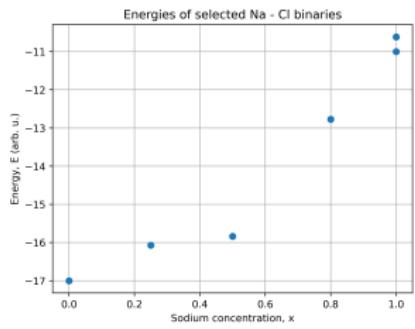
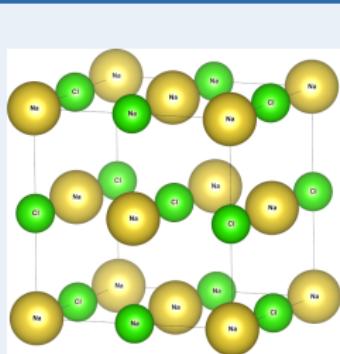
Approach



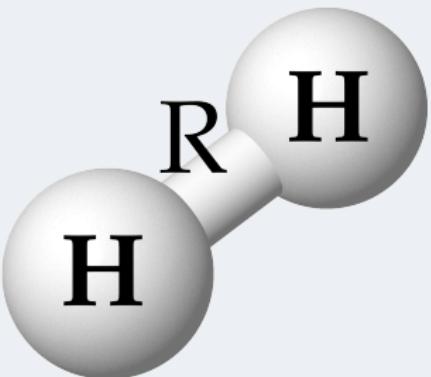
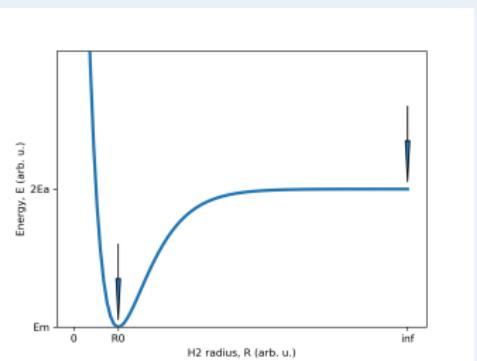
Energy of $H - H$ system



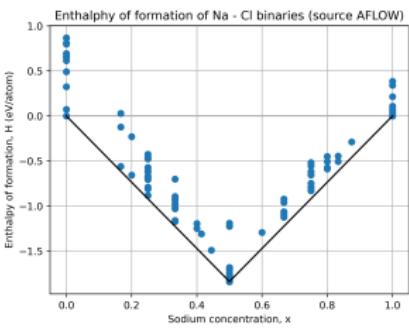
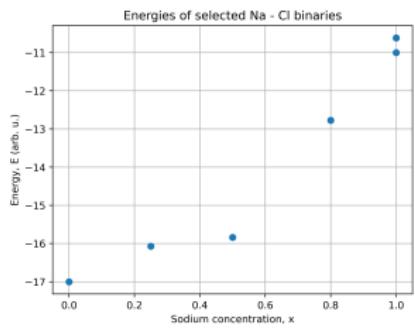
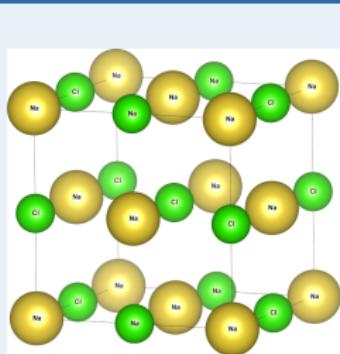
More elements - Energy (Enthalpy) of Formation



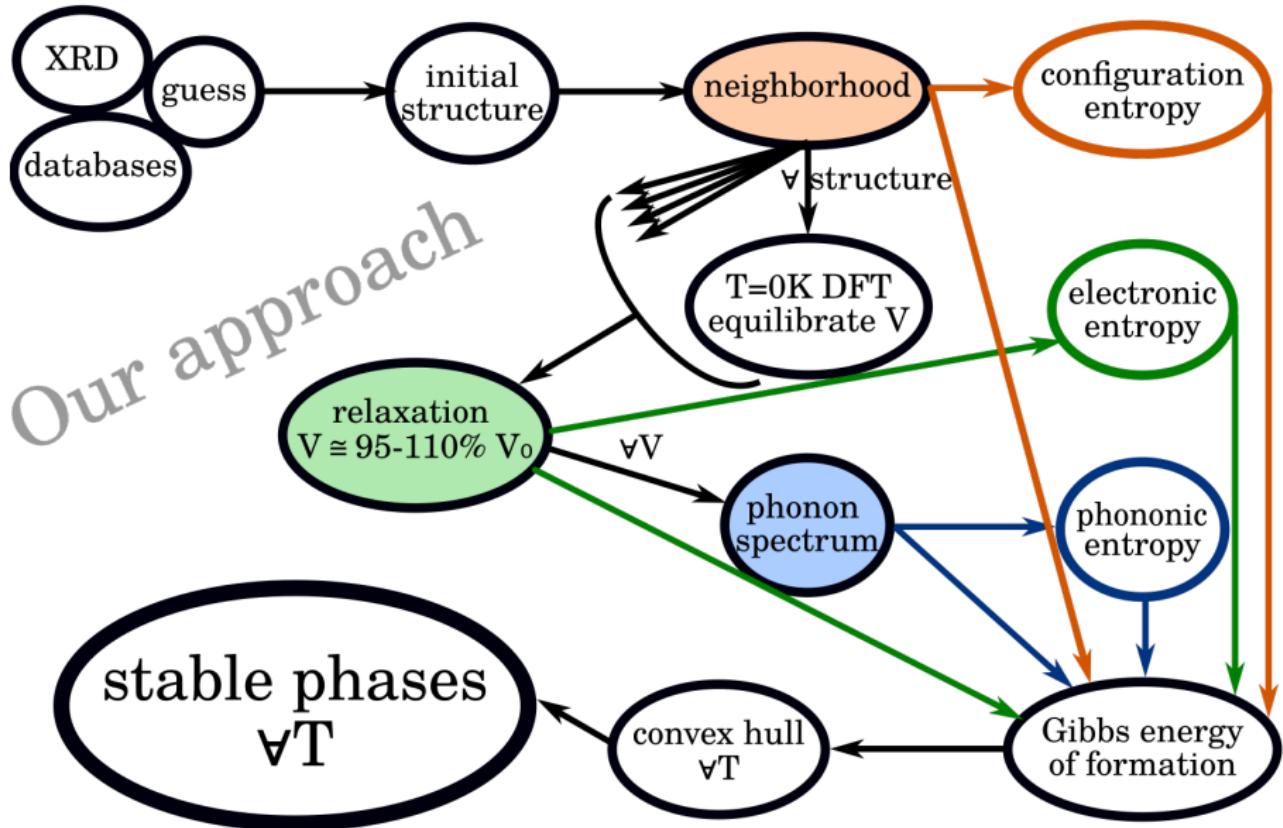
Energy of $H - H$ system



More elements - Energy (Enthalpy) of Formation



Approach



Free energy of formation

Formation of an W_xCr_{1-x} alloy

$$\Delta G_f \equiv G_{W_xCr_{1-x}} - xG_W - (1-x)G_{Cr}$$

$$G_W(p, T) = U_W(V_T^W) + pV_T^W \quad -S_T^W T$$

$$G_{Cr}(p, T) = U_{Cr}(V_T^{Cr}) + pV_T^{Cr} \quad -S_T^{Cr} T$$

$$G_{W_xCr_{1-x}}(p, T) = U_{W_xCr_{1-x}}(V_T^{W_xCr_{1-x}}) + pV_T^{W_xCr_{1-x}} \quad -S_T^{W_xCr_{1-x}} T$$

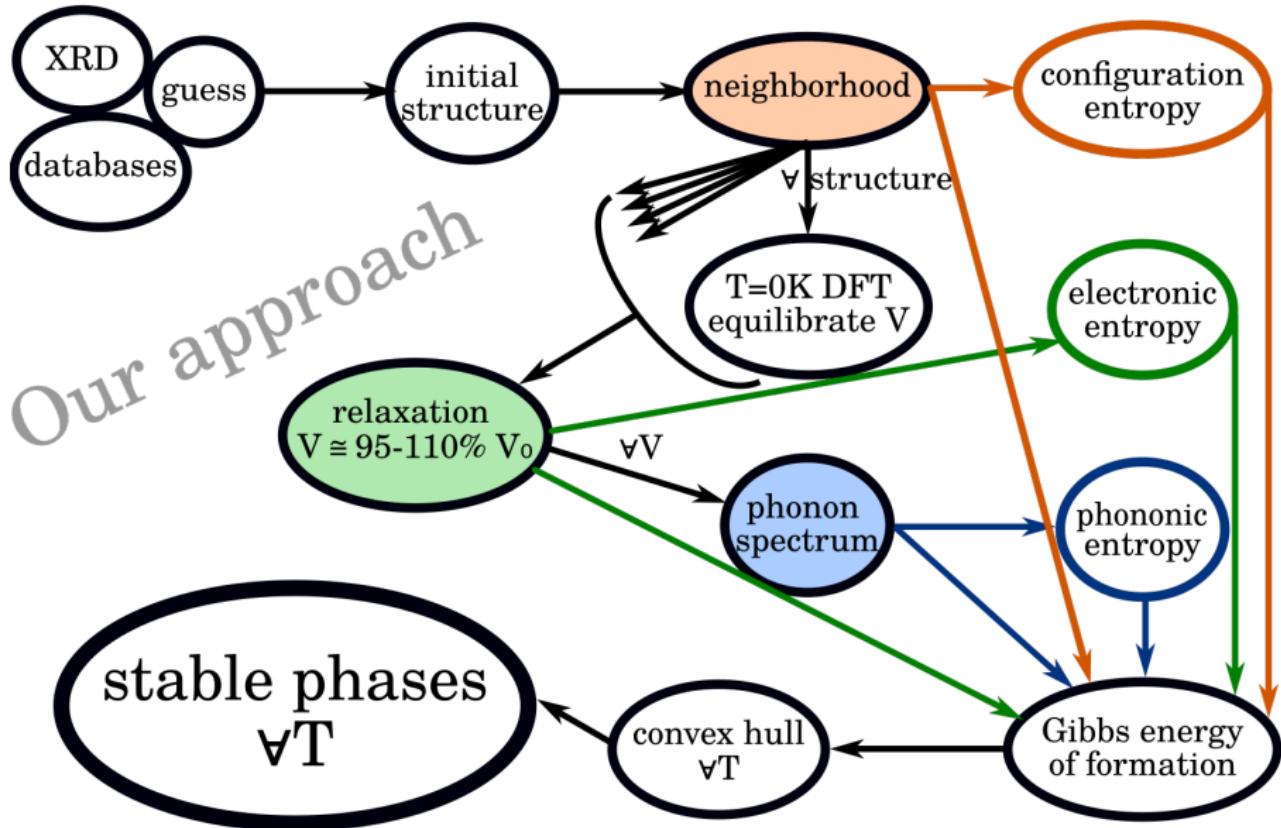
Gibbs entropy $S = S(T) \approx S_{electrons} + S_{phonons} + S_{configuration}$

$$S_{electrons} \equiv -k_B \sum_{\sigma} \int d\epsilon D_{\sigma}(\epsilon) \left(f(\epsilon) \log f(\epsilon) + (1 - f(\epsilon)) \log (1 - f(\epsilon)) \right)$$

$f(\epsilon)$ band structure \rightarrow bosonic Z_b

$$S_{configuration} \approx -k_B(x \log x + (1-x) \log(1-x))$$

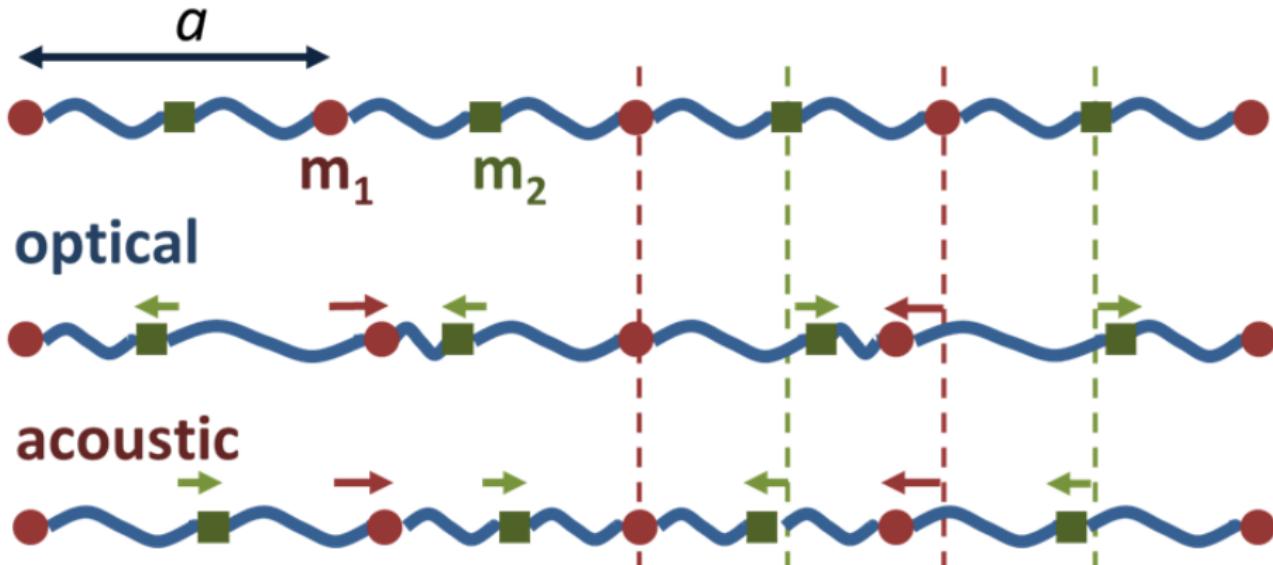
Approach

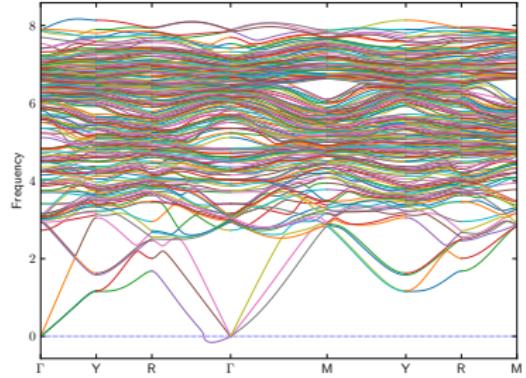
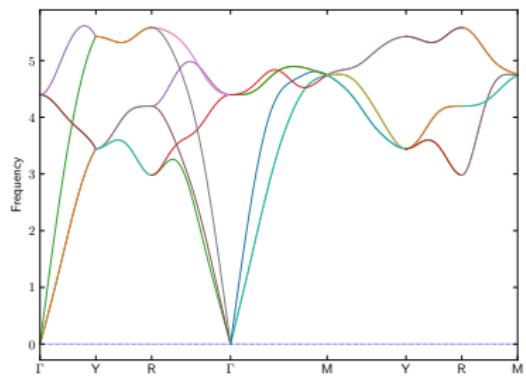
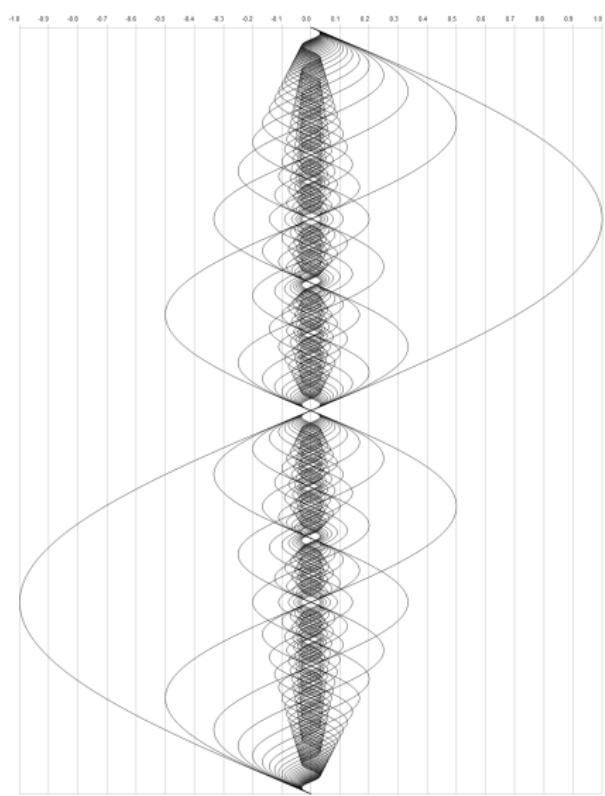


Phonons

Definition (wikipedia)

A collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter.

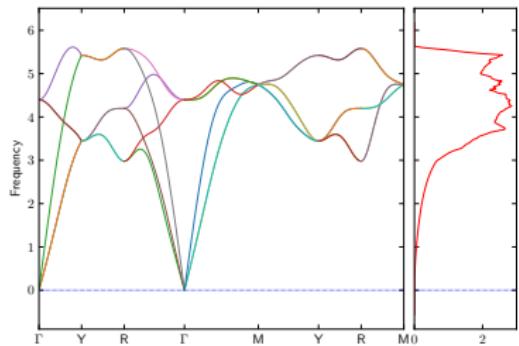




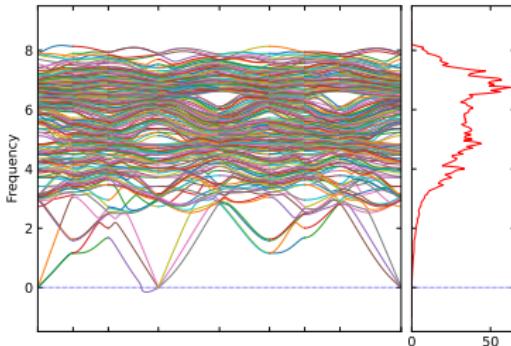
Entropy of phonons

$$S \equiv -\frac{\partial \mathcal{F}}{\partial T} = -\frac{\partial(k_B T \log \mathcal{Z}_B)}{\partial T} = -k_B \sum_{q,\nu} \left[\log(b(\hbar\omega_q^\nu)) - \frac{\hbar\omega_q^\nu}{k_B T} b(\hbar\omega_q^\nu) e^{-\frac{\hbar\omega_q^\nu}{k_B T}} \right]$$

Energy Spectrum



Tungsten

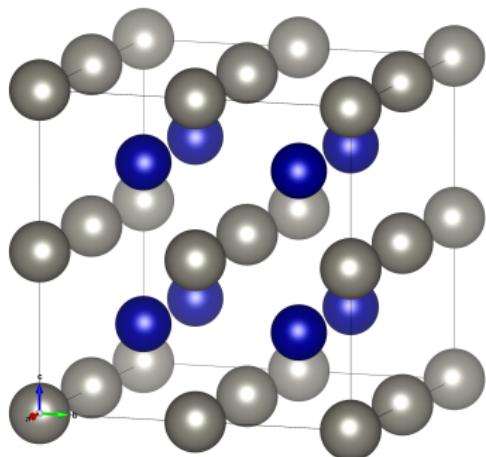


70-30 W-Cr alloy model

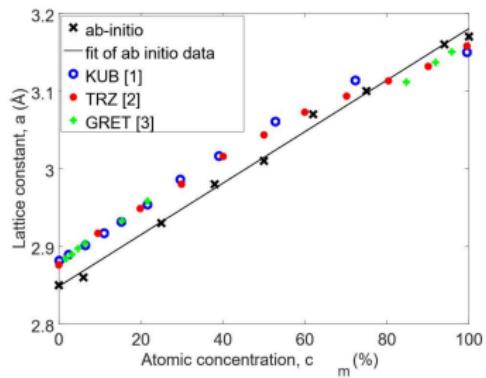
16 atoms, 0K - BSc. Michal Farana

Hypothesis: It is as simple as that.

DFT calculations of arbitrary chosen, symmetric $2 \times 2 \times 2$ supercells.
Perdew–Burke–Ernzerhof (PBE) correlation exchange potential, no
Hubbard U . The calculations in 0K extended via the quasiharmonic
approximation to finite temperature.



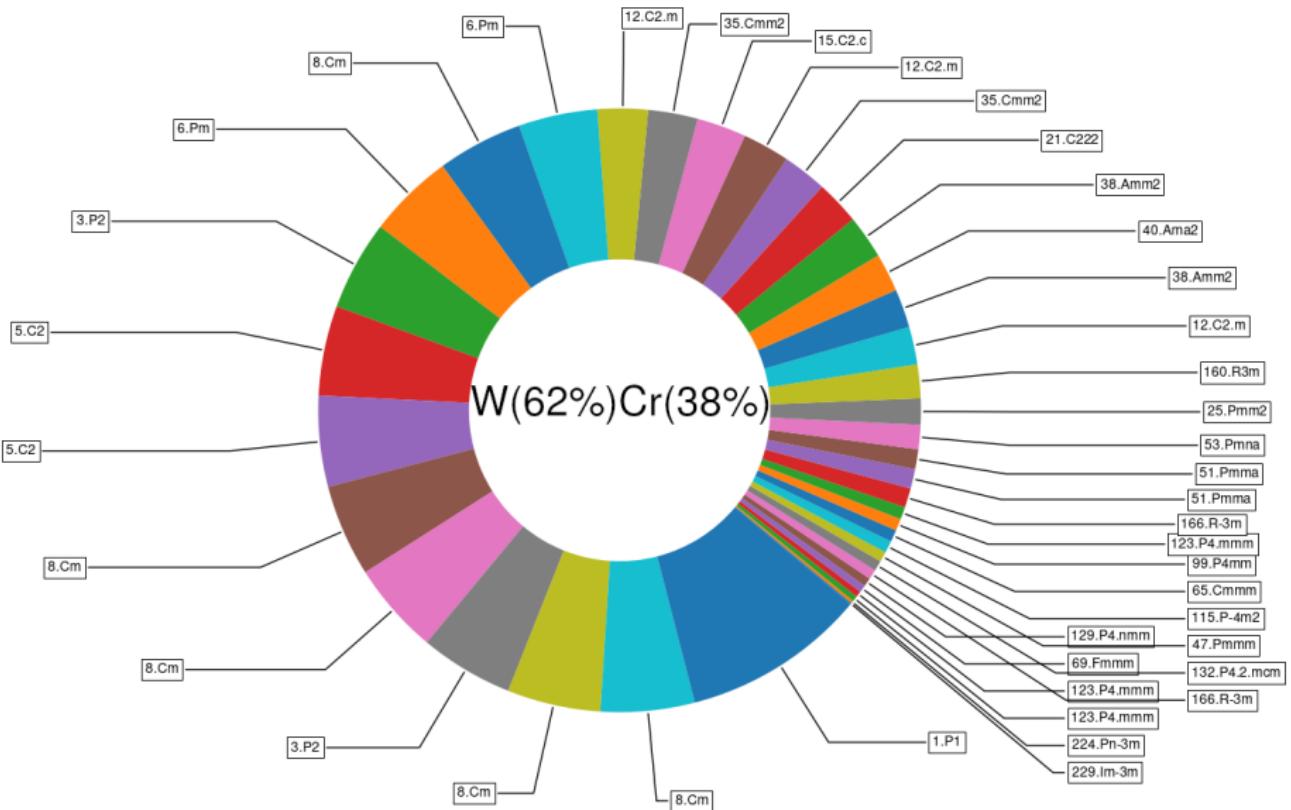
Lattice Constant



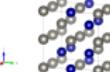
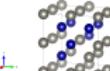
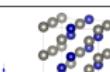
[1] O. Kubaschewski and A. Schneider, "The Systems of Chromium with Tungsten and Molybdenum," Z. Elektrochem., 48, 671-674 ~1942) in German. (Equi Diagram; Experiment

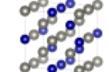
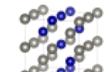
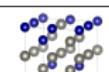
[2] W. Trzebiatowski, H. Płoszek, and J. Łobzowski, "X-Ray Analysis of Chromium-Molybdenum and Chromium-Tungsten Alloys," Anal. Chem., 19, 93-95 (1947). Equi Diagram; Experimental.

[3] H.T. Greenaway, "The Constitutional Diagram of the Chromium-Tungsten System," J. Inst. Met., 80, 589-592 (1951-1952). (Equi Diagram; Experimental.

$W_{62\%}Cr_{38\%}$ 

Exemplary cells $W_{62\%}Cr_{38\%}$

group	E (eV)	cell	
Cm.02 -185.6445		2.2 %	
Cm.04 -185.5567		2.1 %	
P2.01 -185.4322		2.2 %	
Cm.03 -185.3857		2.2 %	
Pm.01 -185.3809		2.0 %	
P2.02 -185.3640		2.1 %	

group	E (eV)	cell	
C2.001 -185.3506		2.1 %	
Pm.02 -185.3131		1.8 %	
Cm.05 -185.3069		2.0 %	
Cm.01 -185.2713		2.2 %	
P1.01 -185.2701		4.3 %	
C2.02 -185.1891		2.1 %	

Special Quasirandom Structures (SQSs)

Goal: alloy vibrations

- Problem: Cell must be finite for the Direct Method.
- Averaging over random ensemble is computationally expensive.
- Even if many cells are taken into account, they still don't reproduce lattice randomness.

Proposition: S. Zunger, *et al.*, Phys. Rev. Lett. **65**, 353 (1990)

A set of symmetric cells reproducing the atomic-type correlations of a fully random alloy.

Neighbor correlation function

Ideal Alloy

For an alloy $A_xB_yC_zD_w\dots$, given $x + y + z + w = 1$, two randomly selected atom have a probability of

$$P = x^2 + y^2 + z^2 + w^2$$

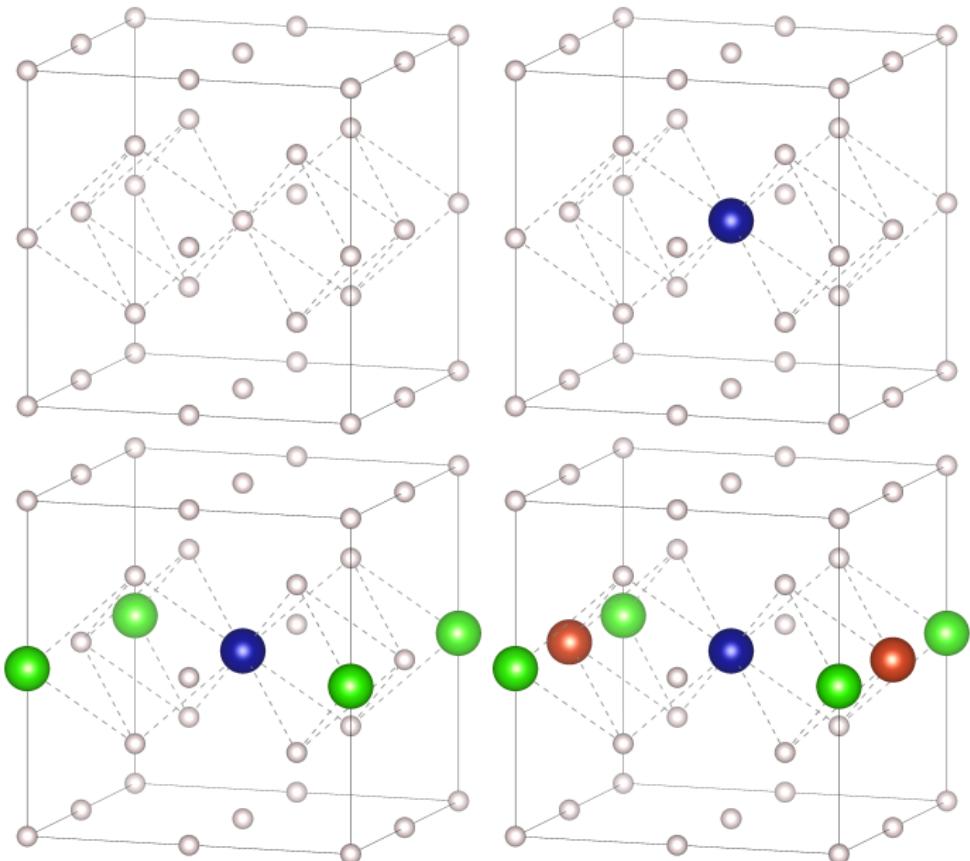
to be of the same element.

Finite model

The property above is true only for infinite models. For the finite one we propose a local two-atom correlation function

$$C_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are the same elements} \\ 0 & \text{if not} \end{cases}$$

Coloring nodes



Correlation function

Finite model - correlation function

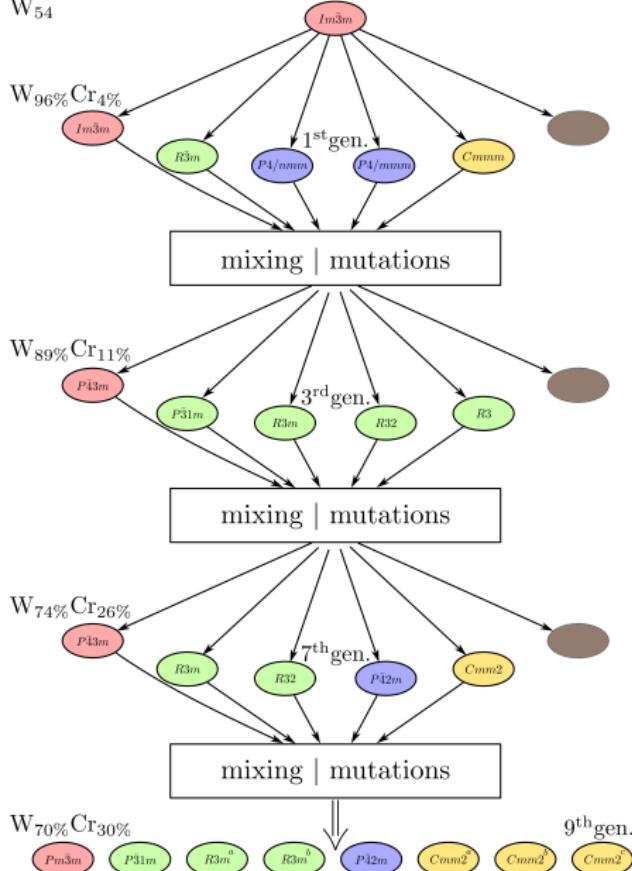
We can now define a correlation function for a coordination zone

$$\mathcal{C}_n = \frac{1}{N} \sum_{i(n)} C_{0i},$$

and an error function

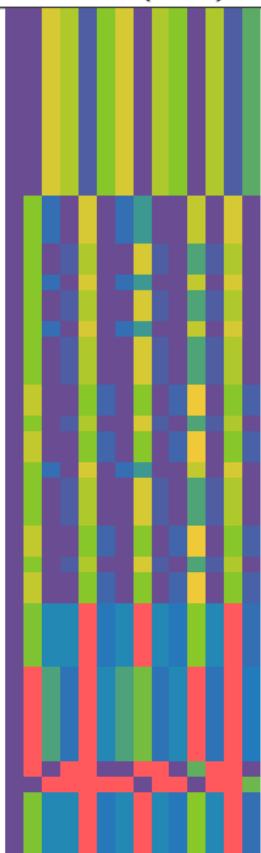
$$\mathcal{E} = \sum_n \mathcal{A}_n (\mathcal{C}_n - P)^2,$$

where \mathcal{A}_n is a decaying function depending on the range of the interactions in the system.

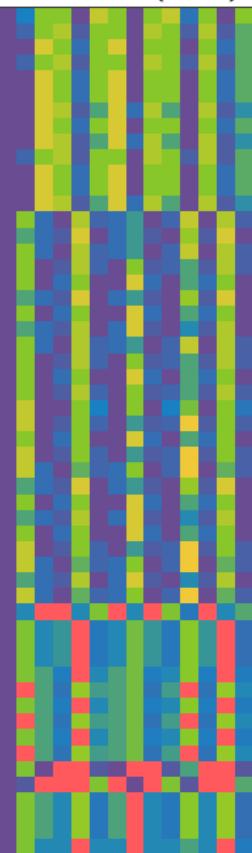
W₅₄

cubic	orthorhombic
<i>Im3m</i>	<i>Cmmm</i>
<i>Pm3m</i>	<i>Cmm2</i>
<i>P43m</i>	<i>Pmm2</i>
tetragonal	trigonal
<i>R3m</i>	<i>I4/mmm</i>
<i>P31c</i>	<i>P4/nmm</i>
<i>P31m</i>	<i>P4/mmm</i>
<i>R3m</i>	<i>P42m</i>
<i>R32</i>	
<i>Cmm2</i>	

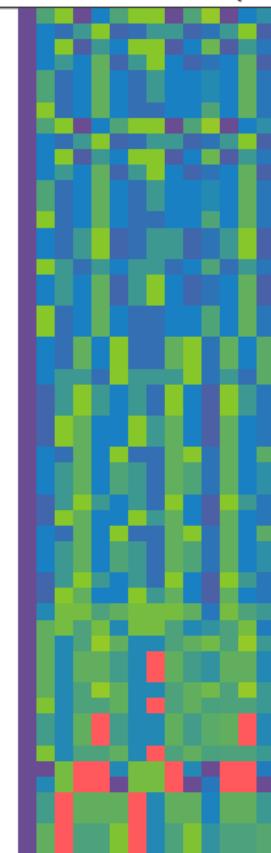
cubic (221)



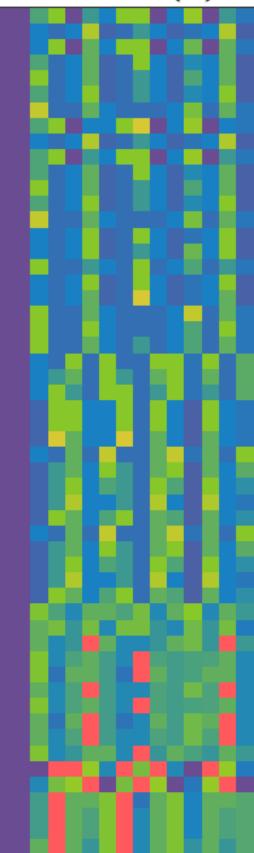
trigonal (160)

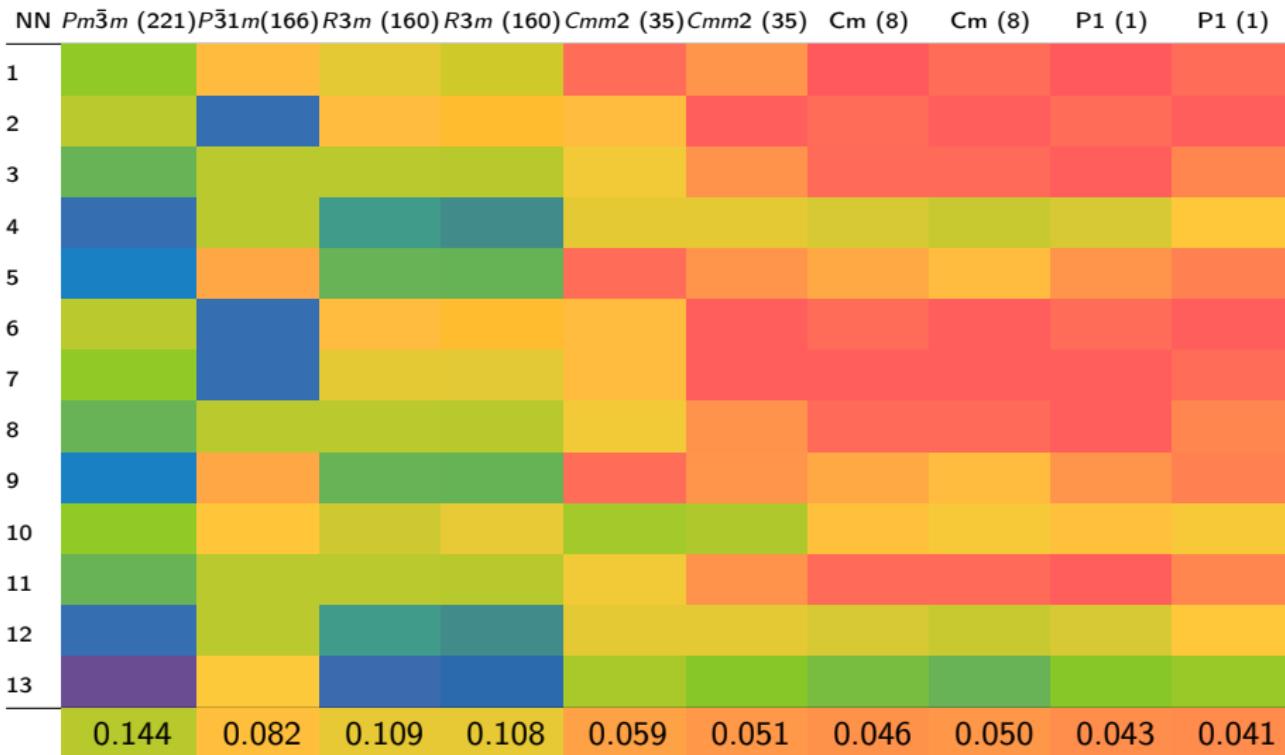


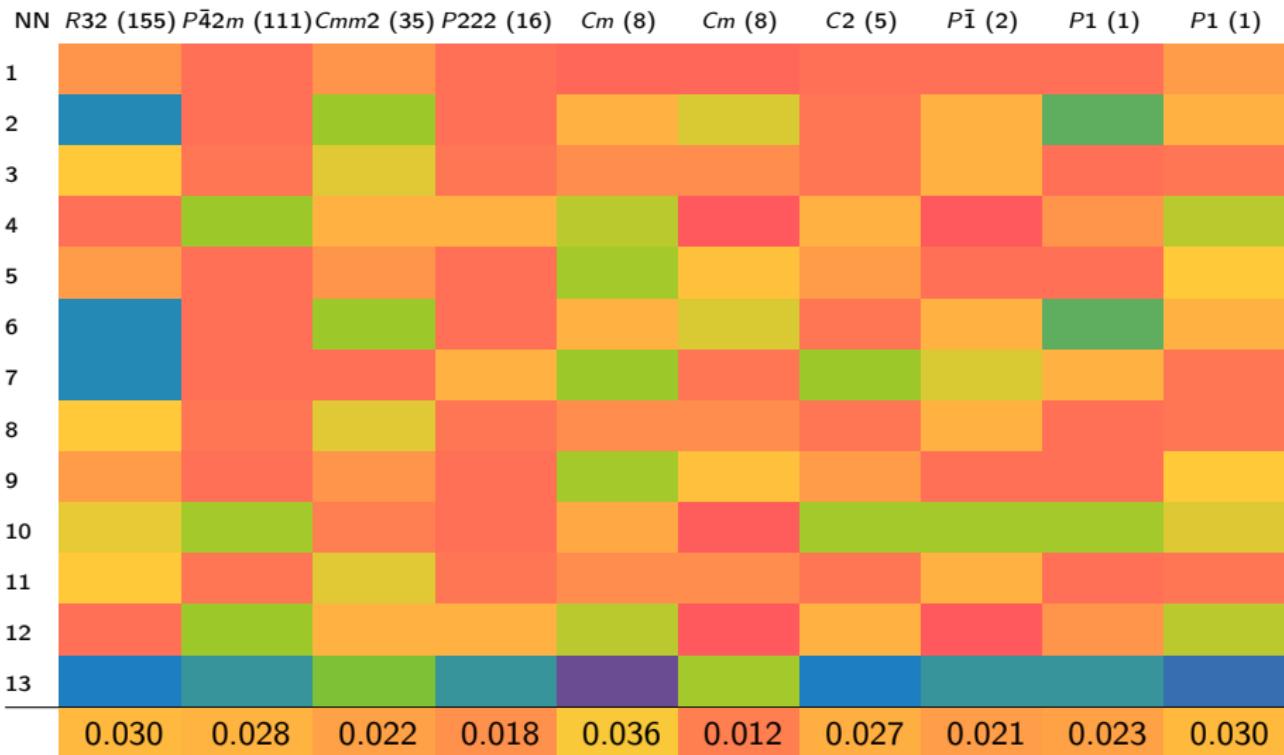
orthorhombic (35)



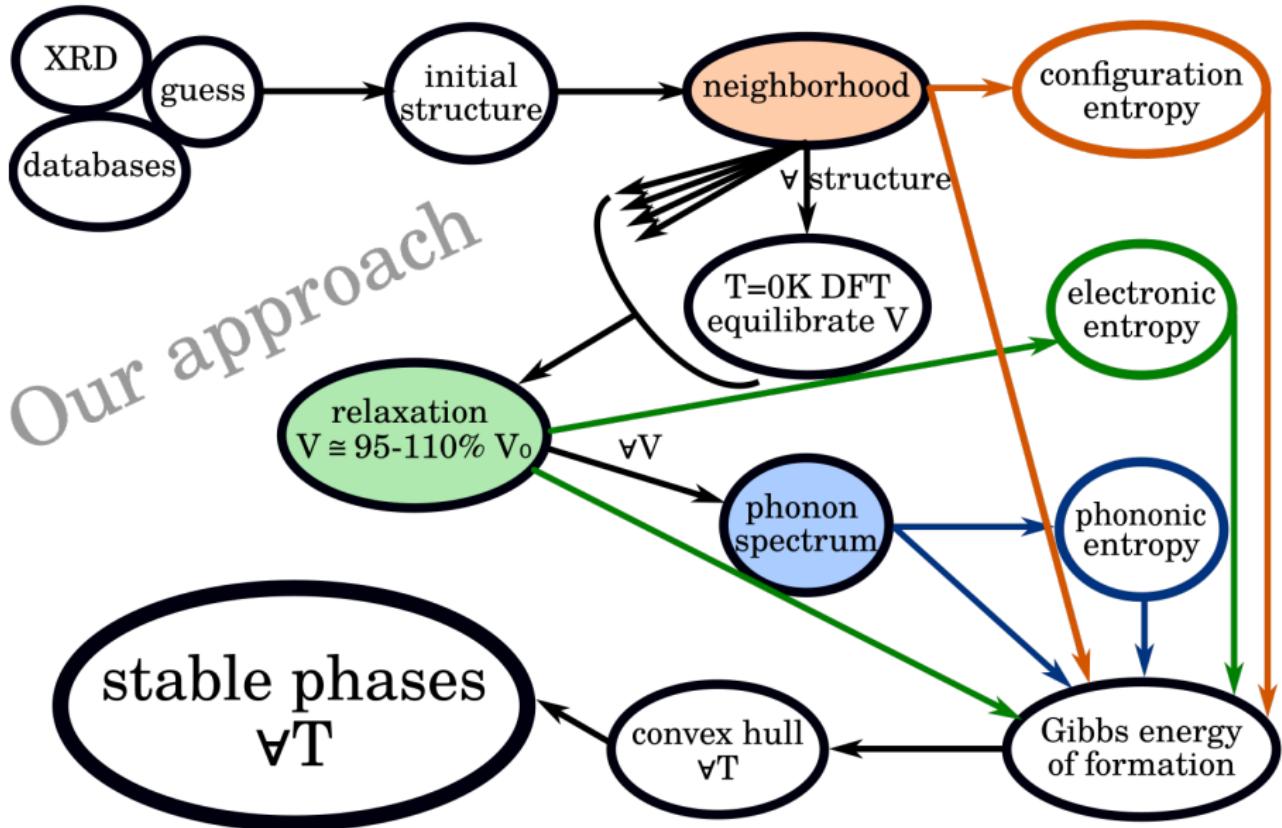
triclinic (1)



Error function $W_{70\%}Cr_{30\%}$ 

Error function: W_{81%}Cr_{19%}

Approach



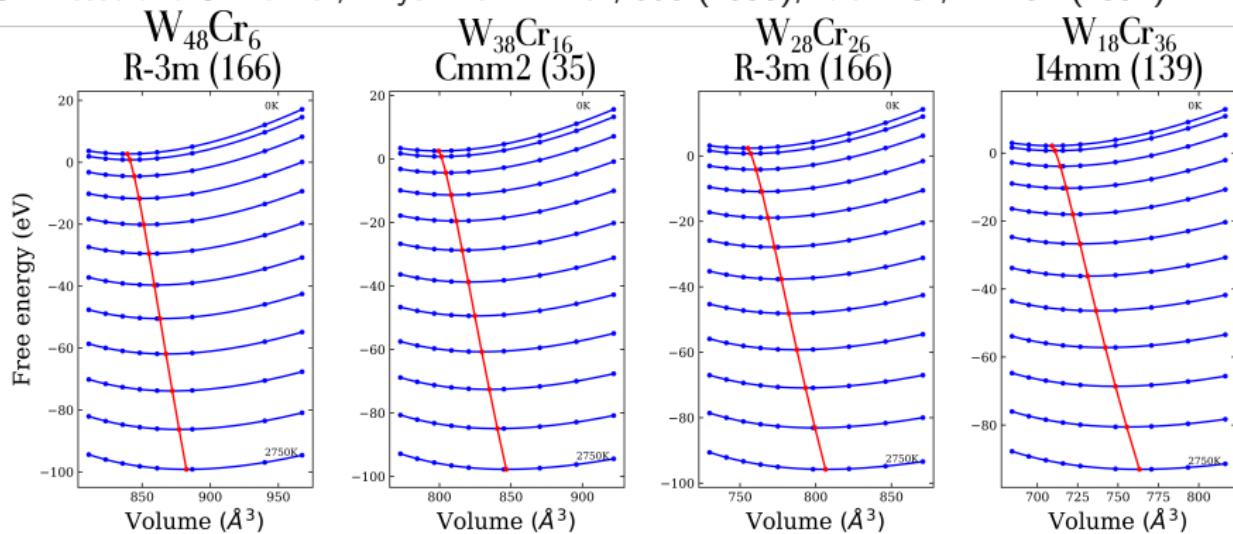
Quasiharmonic approximation

Method

Electronic calculations → Dynamic calculations → $\mathcal{F} = U - ST$ → Optimize $\forall T$ → thermal properties

electronic structure: Vienna ab-initio Software Package (VASP)

G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993); ibid. **49**, 14 251 (1994)



phonon spectra: phonopy A. Togo and I. Tanaka, Scr. Mater., **108**, 1-5 (2015)

Free energy of formation

Formation of an W_xCr_{1-x} alloy

$$\Delta G_f \equiv G_{W_xCr_{1-x}} - xG_W - (1-x)G_{Cr}$$

$$G_W(p, T) = U_W(V_W(T)) + pV_W(T) - (S_W^{electrons} + S_W^{phonons})T$$

$$G_{Cr}(p, T) = U_{Cr}(V_{Cr}(T)) + pV_{Cr}(T) - (S_{Cr}^{electrons} + S_{Cr}^{phonons})T$$

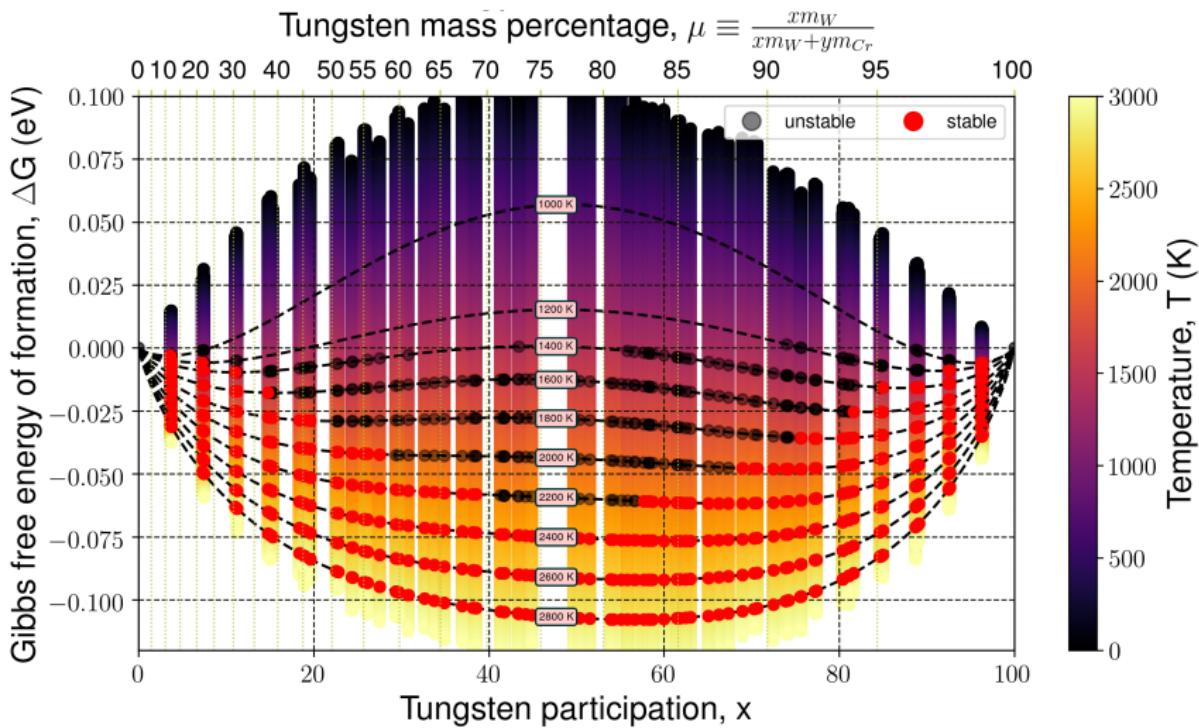
$$G_{W_xCr_{1-x}}(p, T) = U_{W_xCr_{1-x}}(V_{W_xCr_{1-x}}(T)) + pV_{W_xCr_{1-x}}(T) \\ - (S_{W_xCr_{1-x}}^{electrons} + S_{W_xCr_{1-x}}^{lattice dynamics} + S_{W_xCr_{1-x}}^{configuration})T$$

Calculations

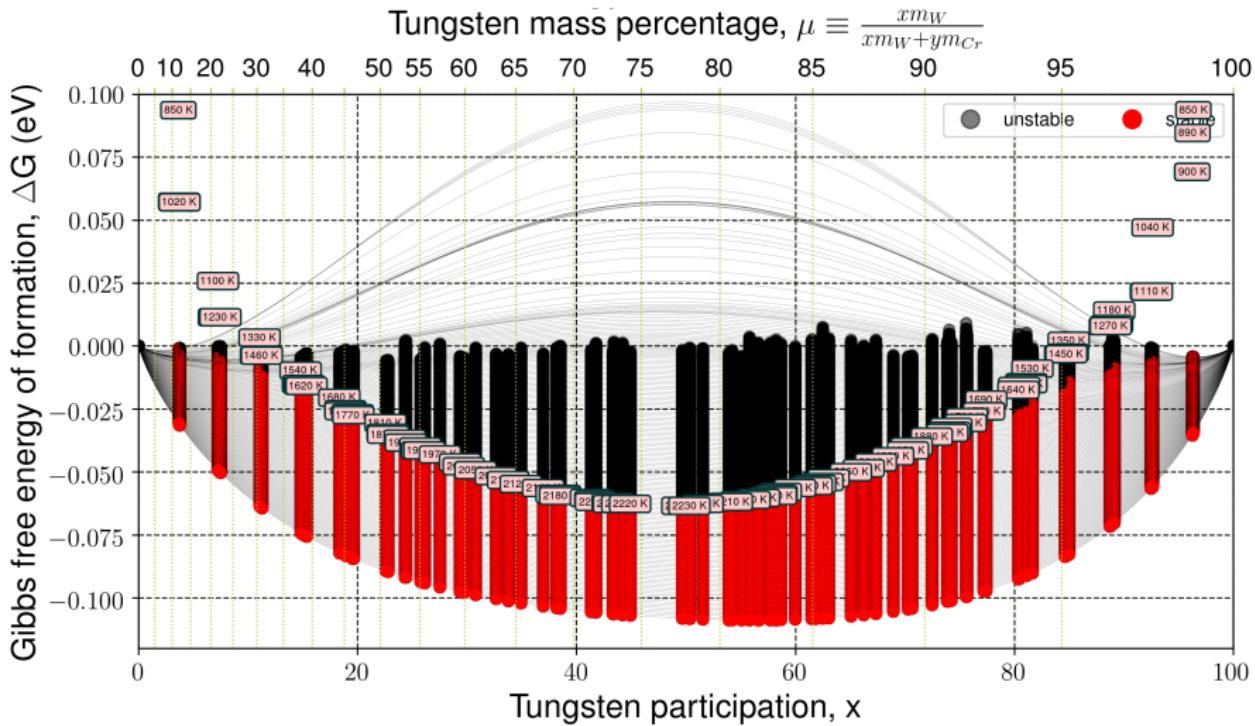
$$S_{W_xCr_{1-x}}^{electrons} \quad S \approx \frac{\pi^2 D(E_f)}{3} k_B^2 T$$

$$S_{W_xCr_{1-x}}^{lattice dynamics} \quad \mathcal{Z} \equiv \sum_{\mu} e^{-\frac{\hbar\omega_{\mu}}{k_B T}} \rightarrow S = -k_B \sum_{\nu} p_{\nu} \log(p_{\nu})$$

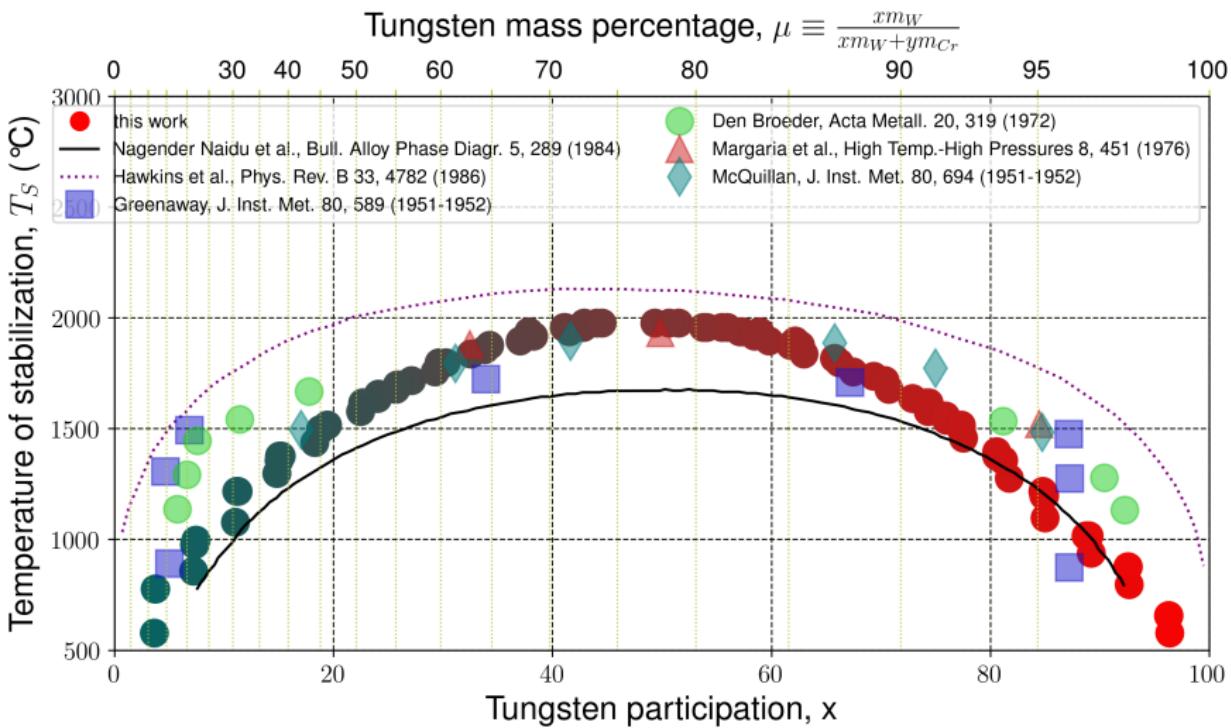
$$S_{W_xCr_{1-x}}^{configuration} \quad S \approx -k_B(x \log x + (1-x) \log(1-x))$$



Gibbs energy of formation for different, realistic compositions in temperature range from 0K (black) to 3000K (yellow). The isothermic lines (dashed) show the points on (red) and off (black) the convex hull.

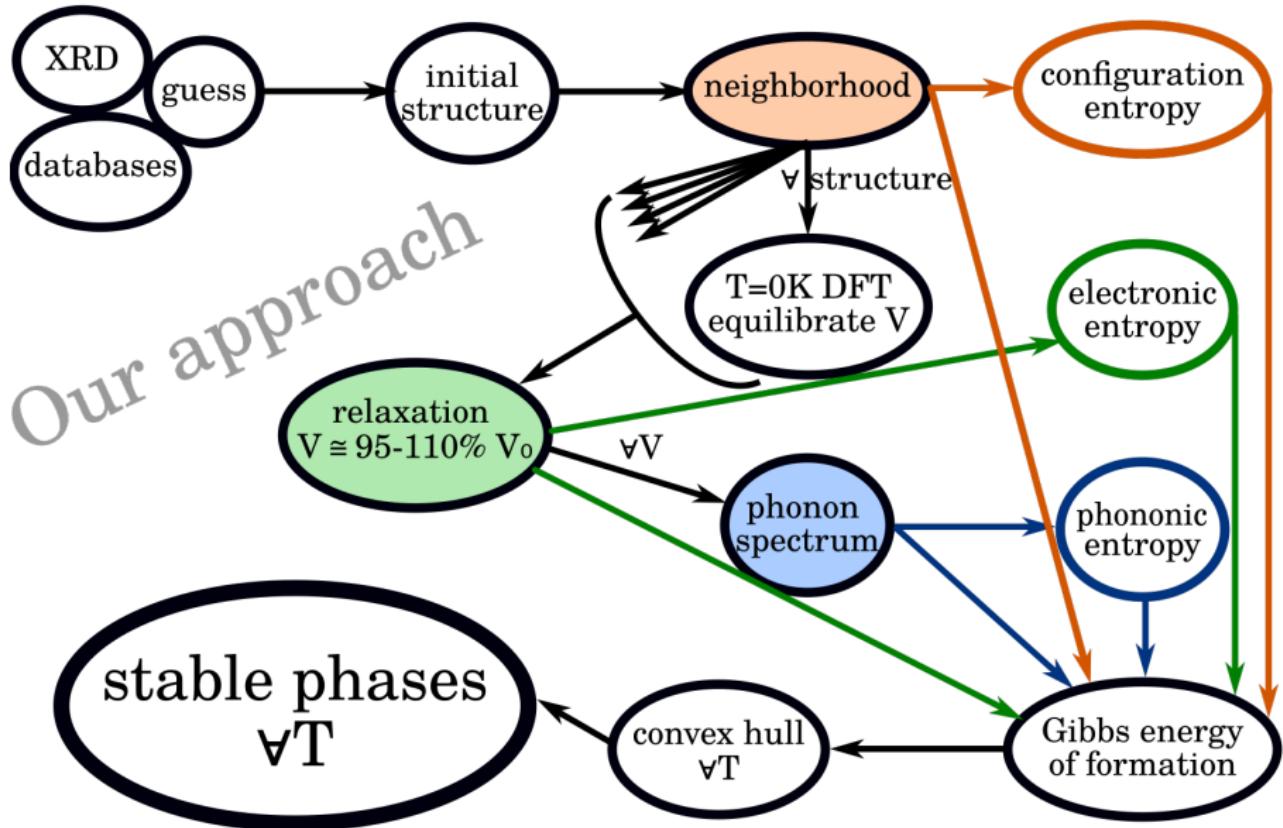


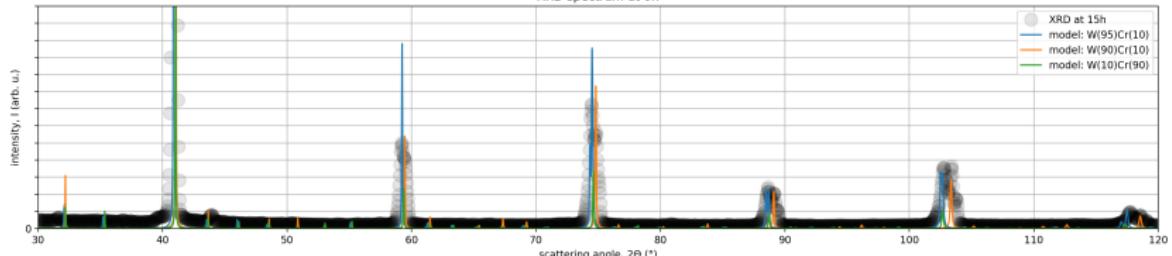
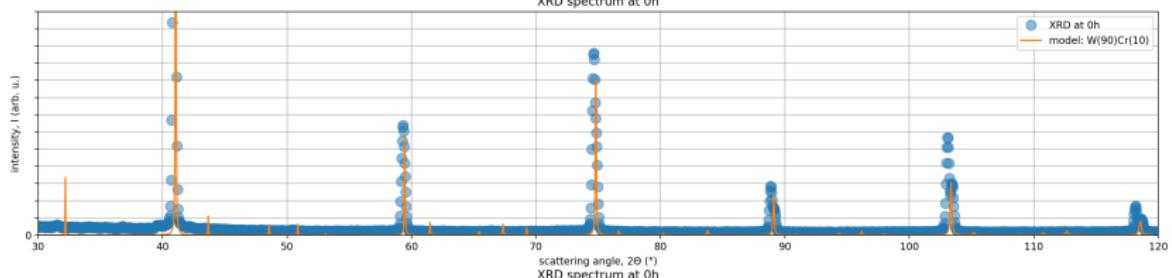
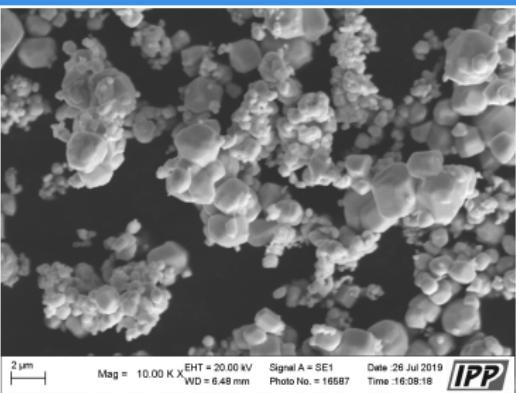
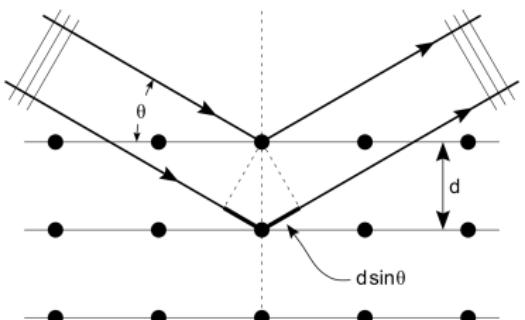
Gibbs energy of formation for different, realistic compositions. The isothermic lines (dashed) show the points on (red) and off (black) the convex hull. Labels correspond to stabilization temperature T_S (K).



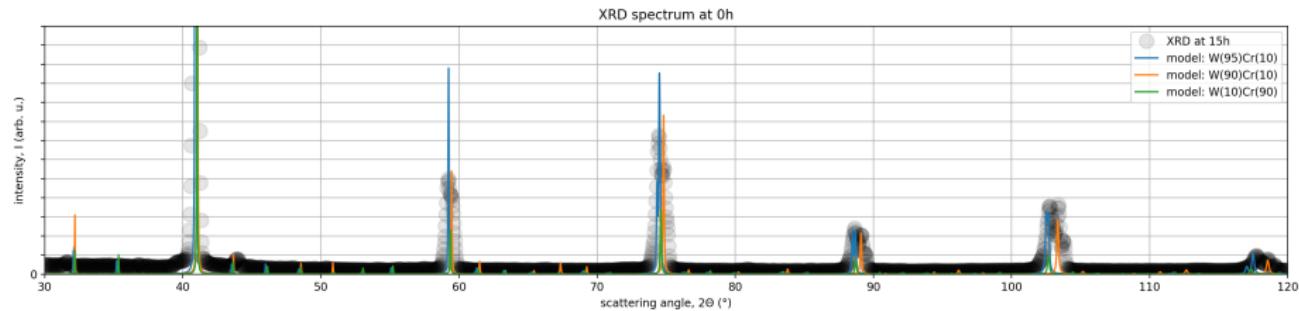
The W-Cr composition - temperature phase diagram. Comparison of our results (green-to-red circles) with other theoretical (lines) and experimental (points) works.

Approach



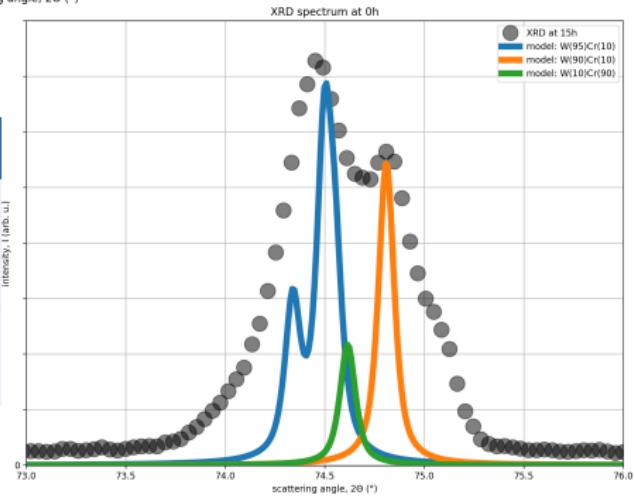


XRD spectra of composite states



XRD composition

	W90Cr10	W95Cr5	W26Cr74
0 h wt %	97.7	∅	∅
15 h wt %	29.6	66.0	2.7
vol. %	34.5	35.9	15.5
alloy %	40.2	41.8	18.0



Hooke's law for a 3D lattice

Harmonic Approximation

$$\mathcal{F} = \mathcal{F}_0 + \sum_{i\alpha;j\beta} \Phi_{\alpha\beta}^{ij} u_i^\alpha u_j^\beta + \dots,$$

where \mathcal{F} is free energy, \mathcal{F}_0 a free energy of the equilibrium, and Φ^{ij} a force constant after displacing sites i and j by u_i and u_j respectively.

Symmetry constraints and Voigt notation

$$\vec{\sigma} = \mathbb{C} \vec{\varepsilon} \xrightleftharpoons[\quad]{\mathbb{S} = \mathbb{C}^{-1}} \vec{\varepsilon} = \mathbb{S} \vec{\sigma},$$

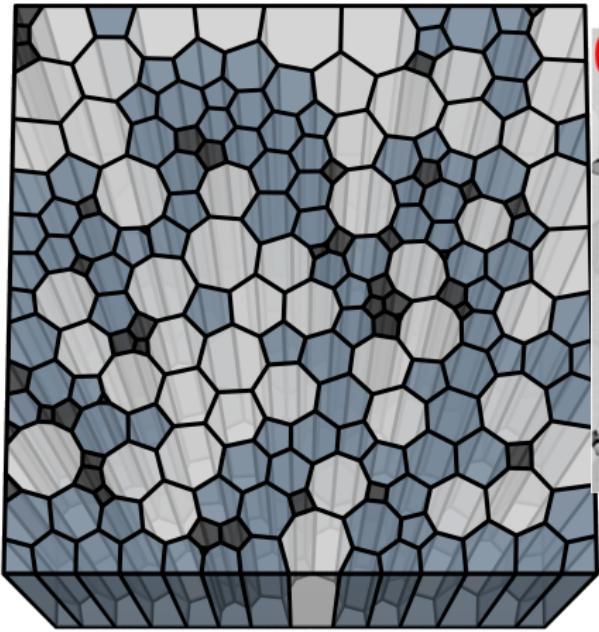
where $\vec{\varepsilon}$ and $\vec{\sigma}$ are the strain and stress vectors in Voigt notation

$$\begin{aligned}\vec{\sigma} &= (\sigma_{xx} \sigma_{yy} \sigma_{zz} \sigma_{xy} \sigma_{yz} \sigma_{zx})^T, \\ \vec{\varepsilon} &= (\varepsilon_{xx} \varepsilon_{yy} \varepsilon_{zz} \varepsilon_{xy} \varepsilon_{yz} \varepsilon_{zx})^T,\end{aligned}$$

and \mathbb{C} and \mathbb{S} are the 6×6 symmetric elastic and compliance tensors.

E. M. Lifshitz, A. M. Kosevich, L. P. Pitaevskii, Course of Theoretical Physics by L. D. Landau and E. M. Lifshitz: Theory of Elasticity (Third Edition), Chapter I - Fundamental equations, Butterworth-Heinemann, 1986, Pages 1-37, ISBN 9780080570693

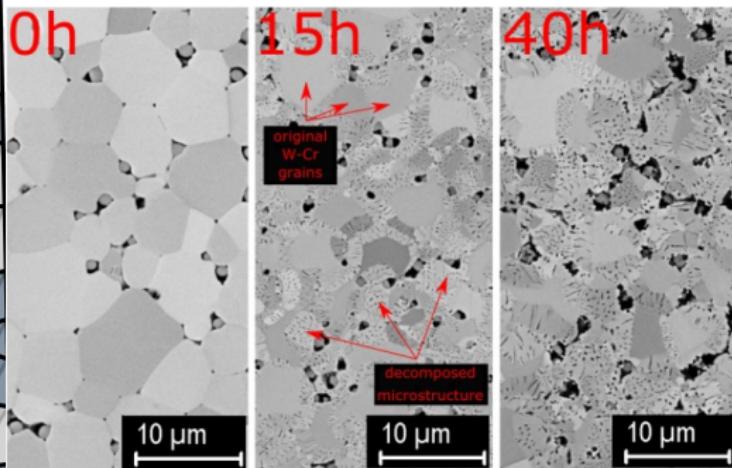
Rode-like microstructure



W(96)Cr(4)
 W(91)Cr(9)
 W(19)Cr(81)

Simulated rod-like 3D structure: tessellation using neper

<https://neper.info/>

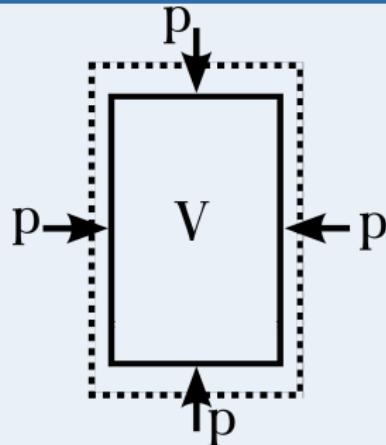


Properties of the composite

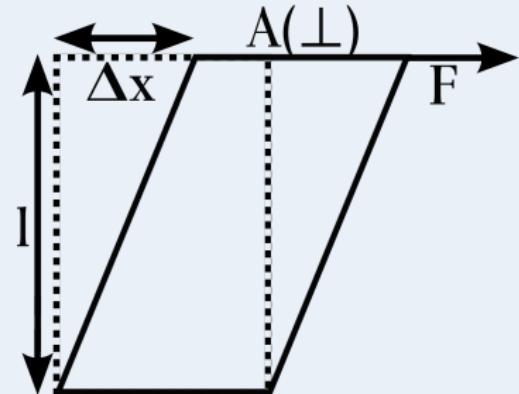
Average over different grains

$$\check{\mathbb{C}} \equiv \frac{1}{N} \sum_{\text{grain,seed}} \mathbb{O}'(\text{seed}) \mathbb{C} \mathbb{O}(\text{seed})$$

with $\mathbb{O}'(\text{seed}) \neq \mathbb{O}^{-1}(\text{seed})$

Bulk, K and Shear, G Moduli

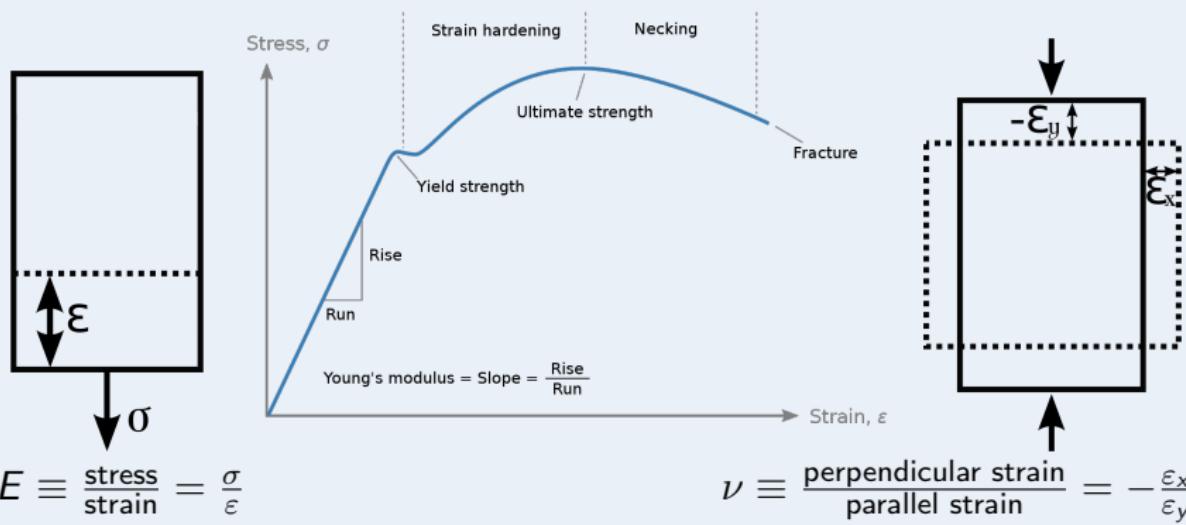
$$K \equiv -V \frac{dp}{dV}$$



$$G \equiv \frac{\text{shear stress}}{\text{shear strain}} = \frac{F}{A} \left(\frac{\Delta x}{l} \right)^{-1}$$

Values

	Diamond	$W_{(90)}Cr_{(10)}$ (exp)	Steel	Aluminium	Rubber
K (GPa)	443	263	160	162	2
G (GPa)	478	133	79	26	0.0006

Young's Modulus, E and Poisson Ratio, ν 

Values

	Diamond	$W_{(90)}Cr_{(10)}$ (exp)	Steel	Aluminium	Rubber
E (GPa)	1210	341	200	68	<0.1
ν		0.284	~0.29	0.32	0.4999

Moduli from Hooke's law

Symmetry constraints and Voigt notation

$$\vec{\sigma} = \mathbb{C} \vec{\varepsilon} \xleftrightarrow{\mathbb{S} = \mathbb{C}^{-1}} \vec{\varepsilon} = \mathbb{S} \vec{\sigma},$$

$$\vec{\varepsilon} = (\varepsilon_{xx} \varepsilon_{yy} \varepsilon_{zz} \varepsilon_{xy} \varepsilon_{yz} \varepsilon_{zx})^T.$$

\mathbb{C} and \mathbb{S} are the 6×6 symmetric elastic and compliance tensors.

E. M. Lifshitz, A. M. Kosevich, L. P. Pitaevskii, Course of Theoretical Physics by L. D. Landau and E. M. Lifshitz: Theory of Elasticity (Third Edition), Chapter I - Fundamental equations, Butterworth-Heinemann, 1986, Pages 1-37, ISBN 9780080570693

Cubic system

$$\mathbb{C} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \rightarrow \begin{aligned} K &\equiv \frac{C_{11}+2C_{12}}{3} \\ G &\equiv C_{44} \\ E &\equiv \frac{9KG}{3K+G} \\ \nu &\equiv \frac{3K-2G}{6K+2G} \end{aligned}$$

Elastic moduli: Realistic systems

Voigt Approximation

$$9K \approx C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{23} + C_{31})$$

$$15G \approx C_{11} + C_{22} + C_{33} - (C_{12} + C_{23} + C_{31}) + 4(C_{44} + C_{55} + C_{66})$$

Reuss Approximation

$$\frac{1}{K} \approx S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{23} + S_{31})$$

$$\frac{15}{G} \approx 4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{23} + S_{31}) + 3(S_{44} + S_{55} + S_{66})$$

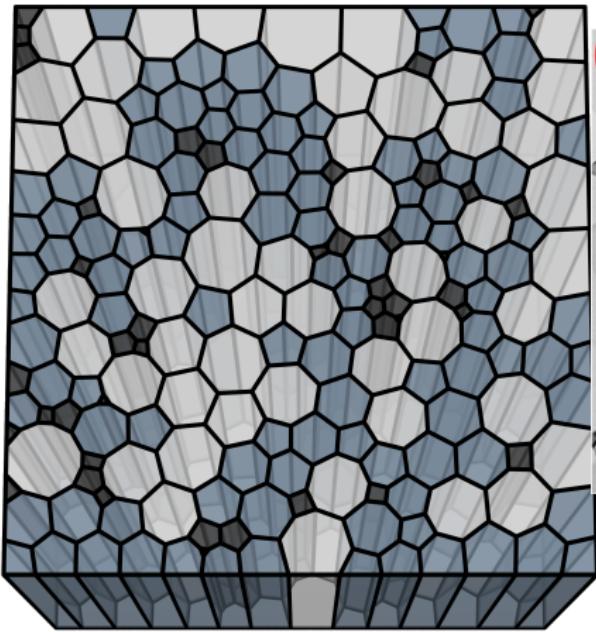
Young modulus and Poisson ratio

$$E \equiv \frac{9KG}{3K+G} \quad \nu \equiv \frac{3K-2G}{6K+2G}$$

C and S calculated via AELAS software:

S. H. Zhang and R. F. Zhang, Comp. Phys. Commun. 220, 403 (2017).

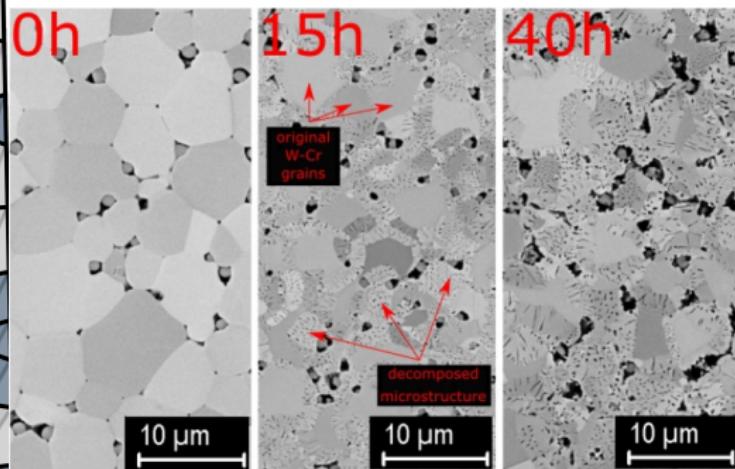
Rode-like microstructure



- W(96)Cr(4)
- W(91)Cr(9)
- W(19)Cr(81)

Simulated rod-like 3D structure: tessellation using neper

<https://neper.info/>



Properties of the composite

Average over different grains

$$\check{\mathbb{C}} \equiv \frac{1}{N} \sum_{\text{grain,seed}} \mathbb{O}'(\text{seed}) \mathbb{C} \mathbb{O}(\text{seed})$$

with $\mathbb{O}'(\text{seed}) \neq \mathbb{O}^{-1}(\text{seed})$

Elastic properties

XRD analysis of the composition (wt %)

	W ₍₉₀₎ Cr ₍₁₀₎	W ₍₉₅₎ Cr ₍₅₎	W ₍₂₆₎ Cr ₍₇₄₎	HfO ₂
0 h	97.7	∅	∅	2.3
15 h	29.6	66.0	2.7	1.7

Elastic properties of materials

	E (GPa)	G (GPa)	K (GPa)	ν
0 h (measured)	340.7(1.0)	132.7(0.3)	262.7(2.0)	0.284(2)
0 h (model 0K)	348	133	300	0.306
0 h (model 1000K)			265	0.279
Δx/x	2 %	0.2 %	1 %	2 %
15 h (measured)	337.7(1.0)	132.3(0.3)	251.8(2.0)	0.276(2)
15 h (model 0K)	354	136	298	0.302
15 h (model 1000K)			263	0.275
Δx/x	5 %	3 %	4 %	0.2 %

Elastic properties @ 700 °C

	Diamond	$W_{(90)}Cr_{(10)}$		Steel	Aluminium	Rubber
		exp	th			
K (GPa)	443	263	265	160	162	2
G (GPa)	478	133	133	79	26	0.0006
E (GPa)	1210	341	348	200	68	<0.1
ν		0.284	0.279	0.27-0.30	0.32	0.4999

Elastic properties of the composite and individual phases @ 700 °C

	15h (exp)	15h (th)	$W_{(96)}Cr_{(4)}$	$W_{(91)}Cr_{(9)}$	$W_{(19)}Cr_{(81)}$	αHfO_2
K (GPa)	252	263	272	265	232	106
G (GPa)	132	136	141	133	116	80
E (GPa)	338	354	366	348	303	192
ν	0.276	0.275	0.281	0.279	0.282	0.198
participation at 15 h			66.0 %	29.6 %	2.7 %	1.7 %

Thank you for your attention!