Materials for application in Fusion Reactors: Determining the elastic properties of single grains in the ultrafine-grained W-Cr composite

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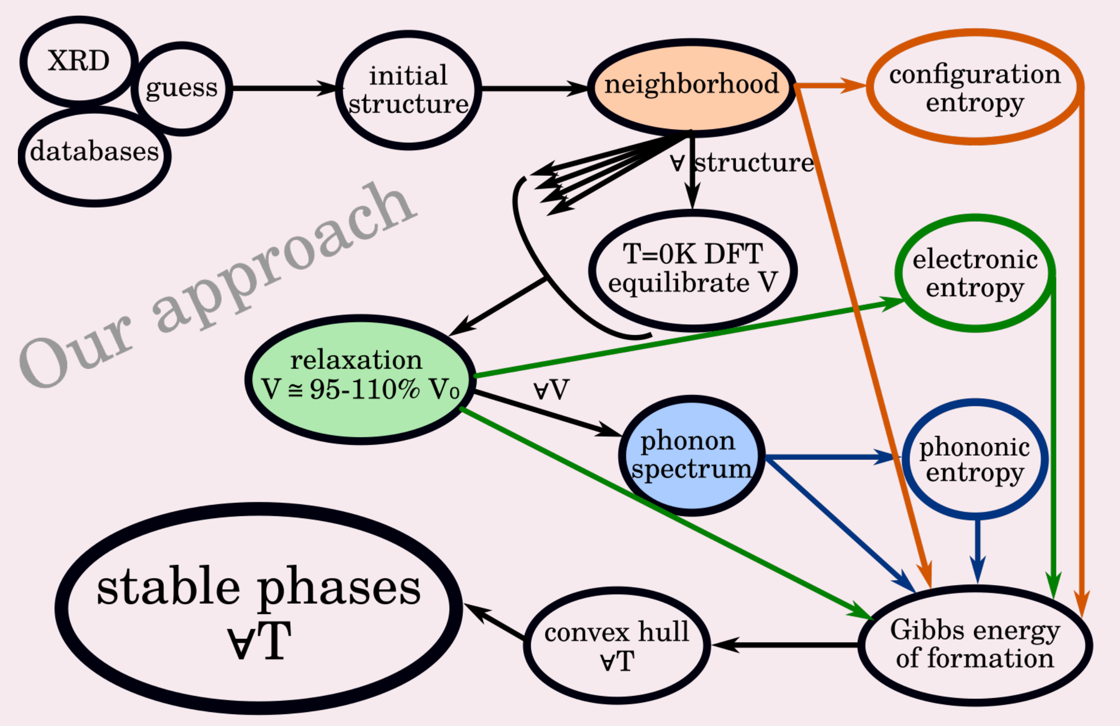
Motivation - to model the experiment

The low oxidation resistance of tungsten limits its operation conditions in high temperetures (e.g., as a so-called first wall of a fusion reactor,) even though its melting point excees 3400 °C. While chromium might be used to enhance oxidation resistance of an alloy, it is difficult to process it with tungsten to an alloy or composite - the system diffuses into a mixture of W-rich and Cr-rich grains. Furthermore, while the elastic properties of a composite microstructure are relatively straightforward in obtaining (e.g., using the resonance ultrasound spectroscopy,) the features of a single, ultrafine grain are not directly measured. There is now the need for an approach to determine these properties by employing large-scale ab-initio modeling techniques (here the Vienna ab-initio software package [1-2] and PhonoPy [3-4].)

Approach



Stability

We model the electronic structure of an alloy in $T \neq 0\,K$ by artificially expand cell's volume. Next, we obtain the temperature dependence of volume by minimizing the Gibbs free energy, whith the entropy being a sum of configuration, electronic, and phononic entropies, i.e.,

$$
\begin{aligned}
S &= S_{\text{configuration}} + S_{\text{electronic}} + S_{\text{phononic}},\\
S_{\text{configuration}} &\equiv -k_B \sum_i x_i \log(x_i), \quad \sum_i x_i \equiv 1\\
S_{\text{electronic}} &\equiv -k_B \sum_\sigma \int d\epsilon DOS_\sigma(\epsilon) \Big(f_{\text{FD}}(\epsilon) \log f_{\text{FD}}(\epsilon) \\
&\qquad + [1 - f_{\text{FD}}(\epsilon)] \log [1 - f_{\text{FD}}(\epsilon)] \Big),\\
S_{\text{phononic}} &\equiv -k_B \sum_{\mathbf{q},\nu} \Big(\log(f_{\text{BE}}(\hbar\omega_{\mathbf{q},\nu})) \\
&\qquad - \hbar\omega_{\mathbf{q},\nu} \beta f_{\text{BE}}(\hbar\omega_{\mathbf{q},\nu}) \exp(-\hbar\omega_{\mathbf{q},\nu}\beta) \Big)
\end{aligned}
$$

Fermi-Dirac distribution $f_{\text{FD}}(E) \equiv \frac{1}{\exp[(E - E_{\text{Fermi}})\beta] + 1}$

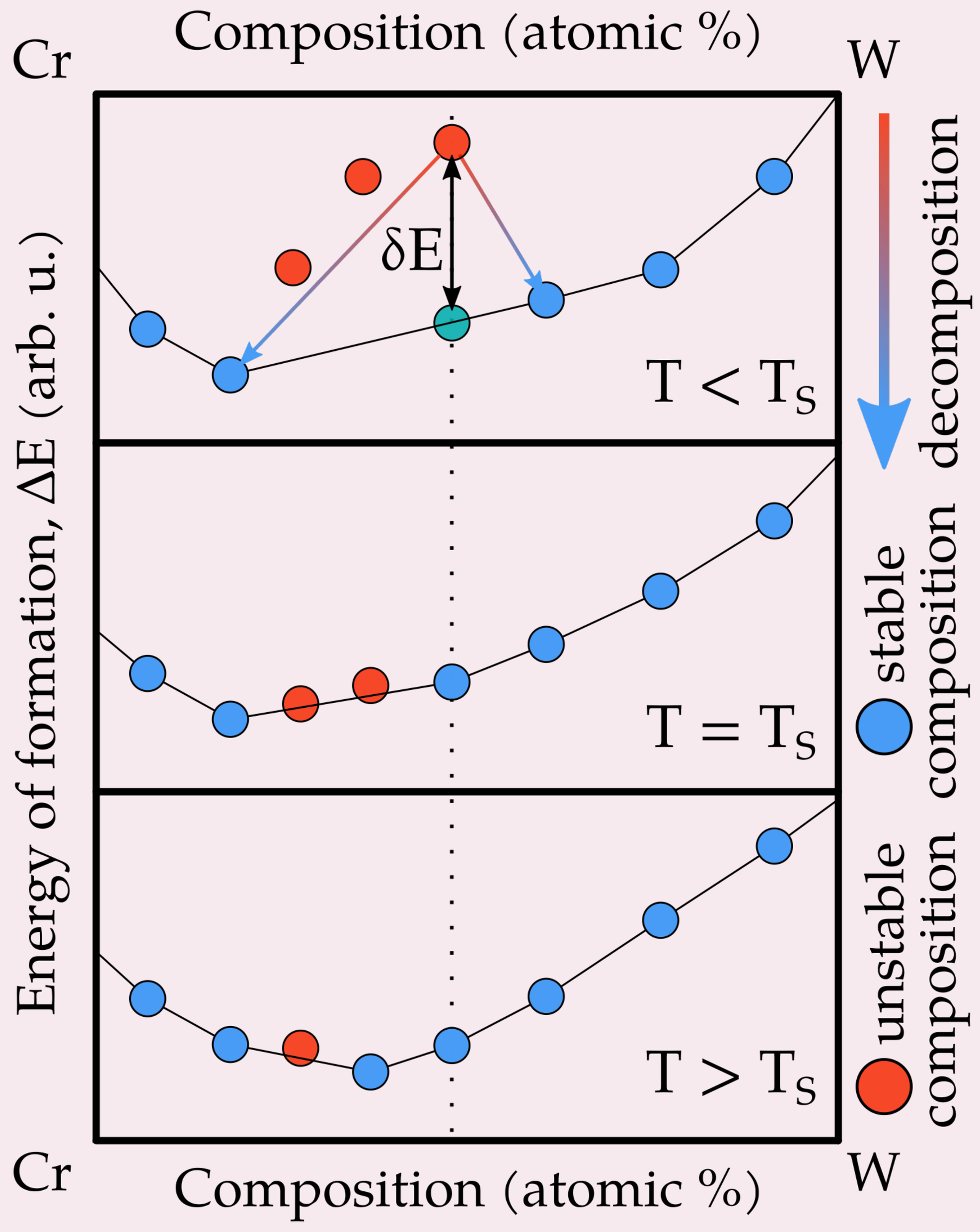
Bose-Einstein distribution $f_{\text{BE}}(E) \equiv \frac{1}{\exp(E\beta) - 1}$

Fermi energy E_{Fermi}

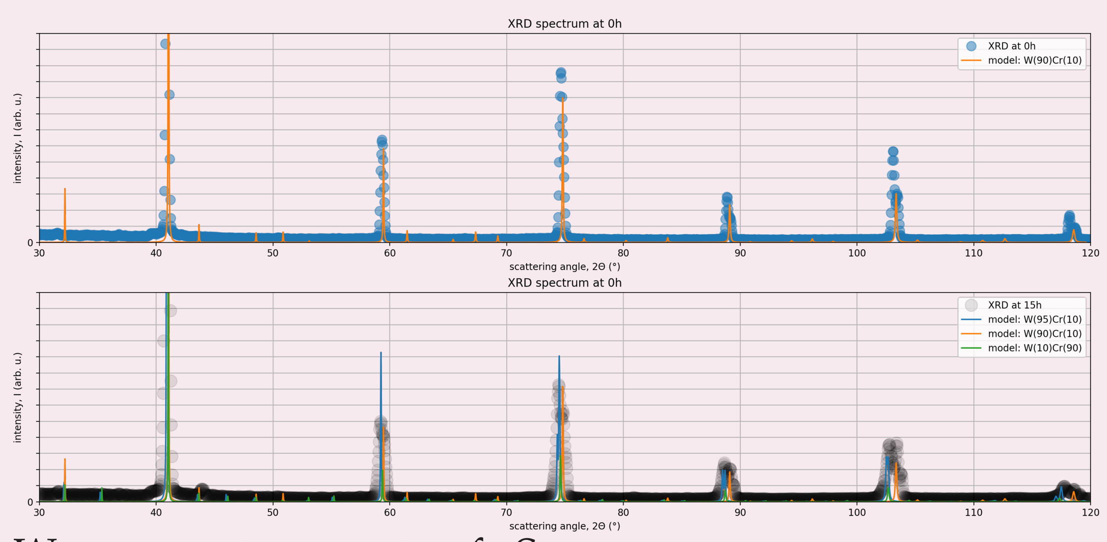
phononic index ν

phononic angular frequency $\omega_{\mathbf{q},\nu}$

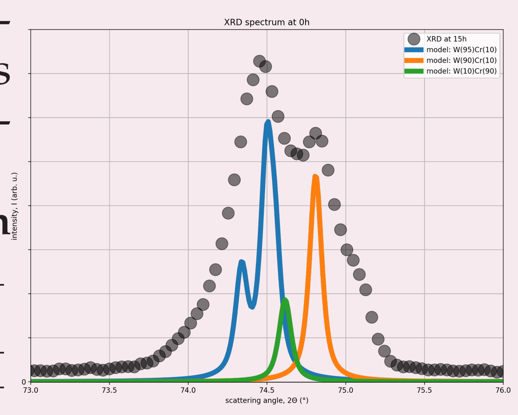
direction in reciprocal space $\mathbf{q}$



Model structures



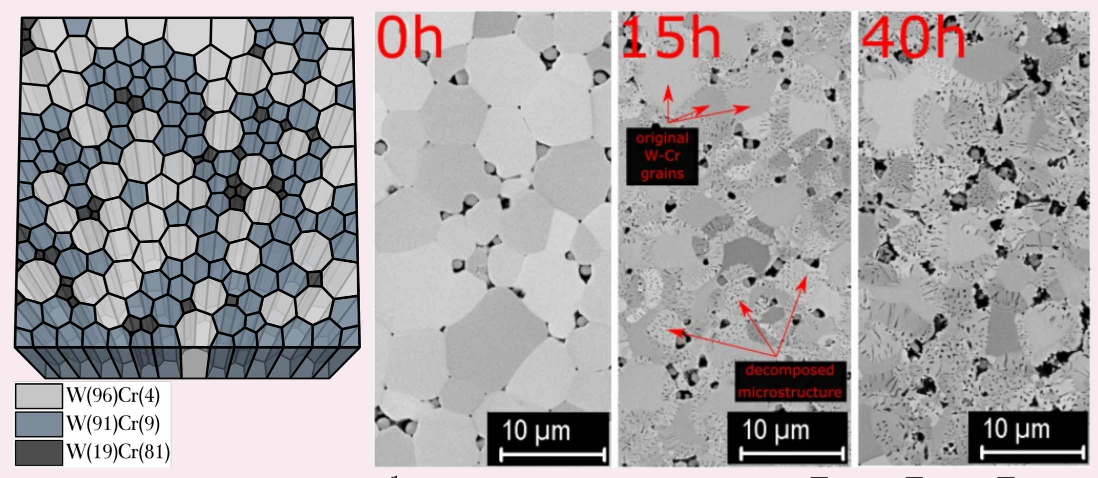
We generate a set of Special Quasirandom Structures (SQS) [5] to model an experimental case.



Before and after decomposition

	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

Grained structure



$$
\begin{aligned}
\mathbb{C} &\to \frac{1}{\mathcal{N}\mathcal{M}} \sum \mathbb{O}_{\hat{z}}(\psi)\mathbb{O}_{\hat{x}}(\theta)\mathbb{O}_{\hat{z}}(\phi)\mathbb{C}_i \mathbb{O}^T_{\hat{z}}(\phi)\mathbb{O}^T_{\hat{x}}(\theta)\mathbb{O}^T_{\hat{z}}(\psi)\\
(\psi,\theta,\phi) &\in \text{a set of } \mathcal{N} \text{ 3-tuples of randomly generated Euler angles}\\
i &\in \text{a set of } \mathcal{M} \text{ grains}
\end{aligned}
$$

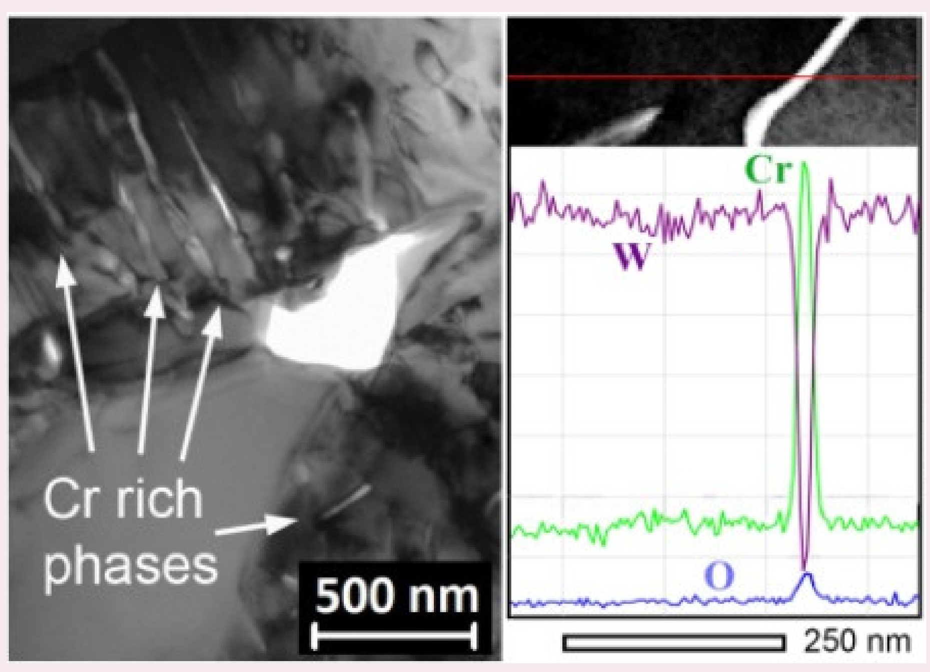
$$
\mathbb{O}_{\hat{z}}(\alpha) \equiv \begin{pmatrix}
\cos(\alpha)^2 & \sin(\alpha)^2 & 0 & 0 & 0 & -\sin(2\alpha)\\
\sin(\alpha)^2 & \cos(\alpha)^2 & 0 & 0 & 0 & \sin(2\alpha)\\
0 & 0 & 1 & 0 & 0 & 0\\
0 & 0 & 0 & \cos(\alpha) & \sin(\alpha) & 0\\
0 & 0 & 0 & -\sin(\alpha) & \cos(\alpha) & 0\\
\frac{\sin(2\alpha)}{2} & \frac{-\sin(2\alpha)}{2} & 0 & 0 & 0 & \cos(2\alpha)
\end{pmatrix}
$$

$$
\mathbb{O}_{\hat{x}}(\alpha) \equiv \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0\\
0 & \cos(\alpha)^2 & \sin(\alpha)^2 & -\sin(2\alpha) & 0 & 0\\
0 & \sin(\alpha)^2 & \cos(\alpha)^2 & \sin(2\alpha) & 0 & 0\\
0 & \frac{\sin(2\alpha)}{2} & \frac{-\sin(2\alpha)}{2} & \cos(2\alpha) & 0 & 0\\
0 & 0 & 0 & 0 & \cos(\alpha) & \sin(\alpha)\\
0 & 0 & 0 & 0 & -\sin(\alpha) & \cos(\alpha)
\end{pmatrix}
$$

Elastic properties of Tungsten-Chromium alloy

Properties at $T = 0\,K$ are calculated using AELAS [6] software, whereas bulk modulus $K = K(T)$ is derived from the Helmholtz energy at given temperature T.

	Young modulus E (GPa)	shear modulus G (GPa)	bulk modulus K (GPa)	Poisson ratio 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)		$\nu \equiv \frac{3K-E}{6K}$	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)		$\nu \equiv \frac{3K-E}{6K}$	263	0.275
Δx/x	5 %	3 %	4 %	0.2 %



	Diamond	$W_{(90)}Cr_{(10)}$ exp	$W_{(90)}Cr_{(10)}$ th	Steel	Rubber	15h exp	15h th	$W_{(96)}Cr_{(4)}$	$W_{(91)}Cr_{(9)}$	$W_{(19)}Cr_{(81)}$	αHfO_2
K (GPa)	443	**263**	**265**	160	2	**252**	**263**	272	265	232	106
G (GPa)	478	**133**	**133**	79	0.0006	**132**	**136**	141	133	116	80
E (GPa)	1210	**341**	**348**	200	<0.1	**338**	**354**	366	348	303	192
ν		**0.284**	**0.279**	0.27-0.30	0.4999	**0.276**	**0.275**	0.281	0.279	0.282	0.198
						participation at 15 h		66.0 %	29.6 %	2.7 %	1.7 %

For details, see our article: Mat. Lett. **304**, 130728 (2021) [7].

Acknowledgments

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