Assessing Short-range order using total scattering and RMC

- methods, challenges and opportunities

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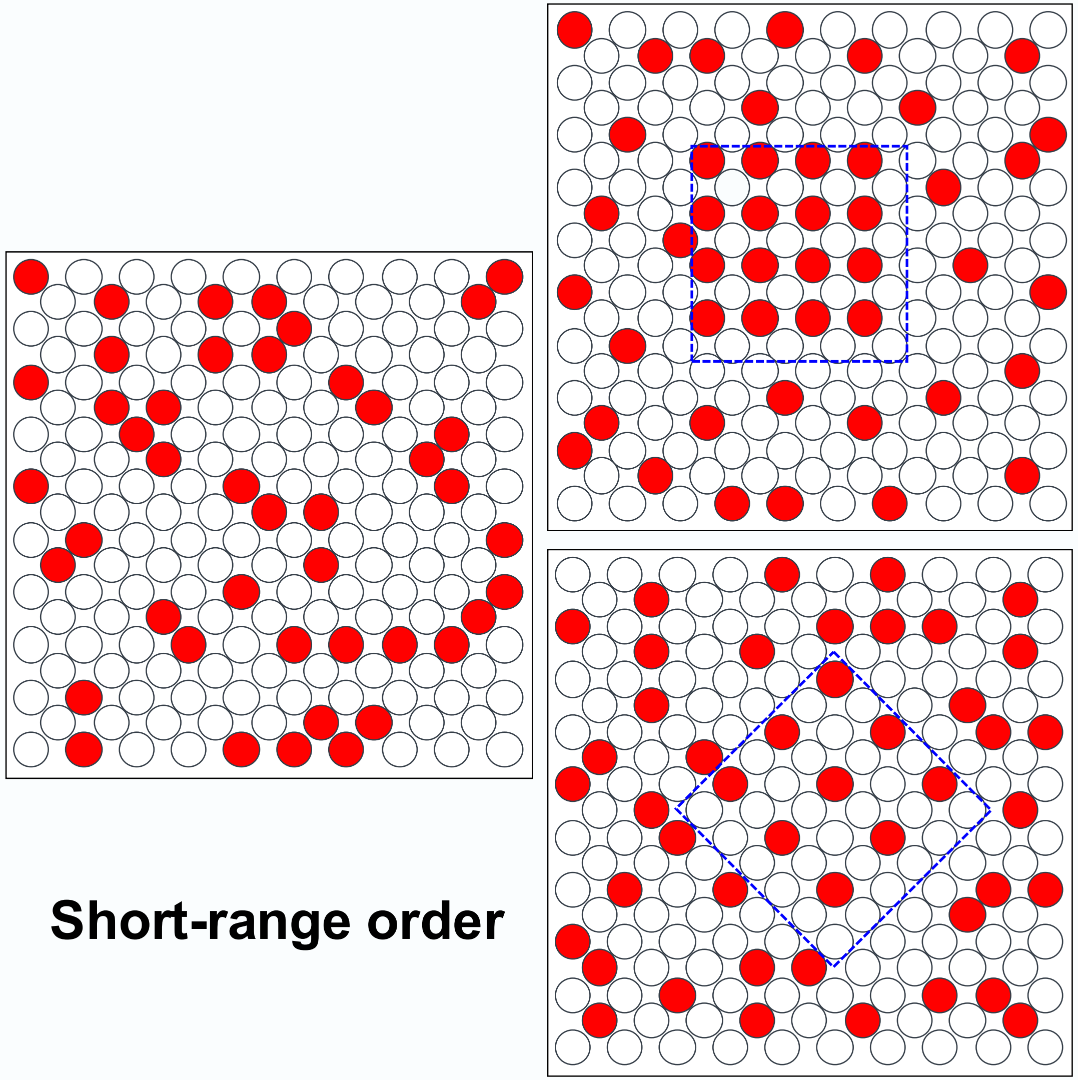
Materials Ordering and Structure : Analysis, Investigation and Characterisation Group

Chapter 1

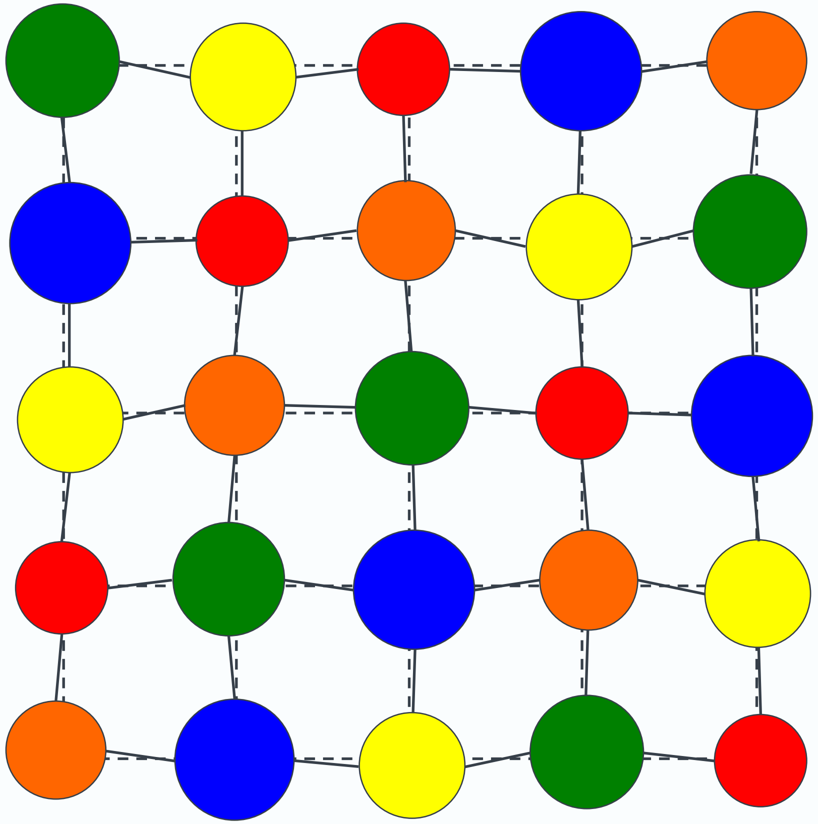
Short-Range Order in alloys

Local Structure in alloy systems

Mosaic



Short-range order

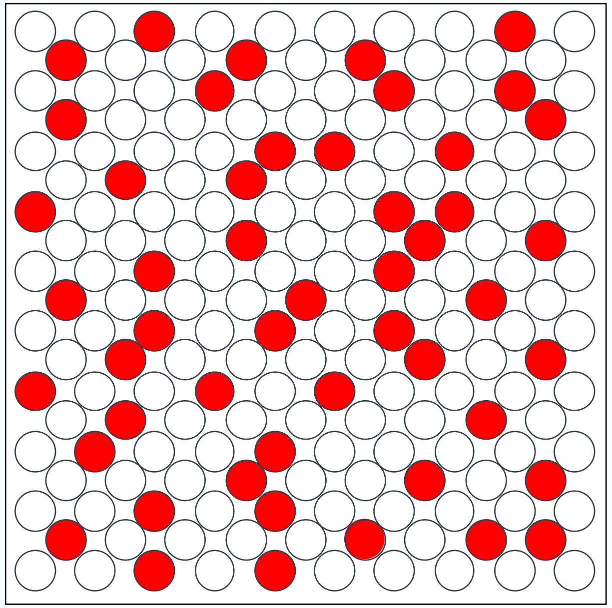


Local lattice distortion

Ordered and Random structures

Mosaic

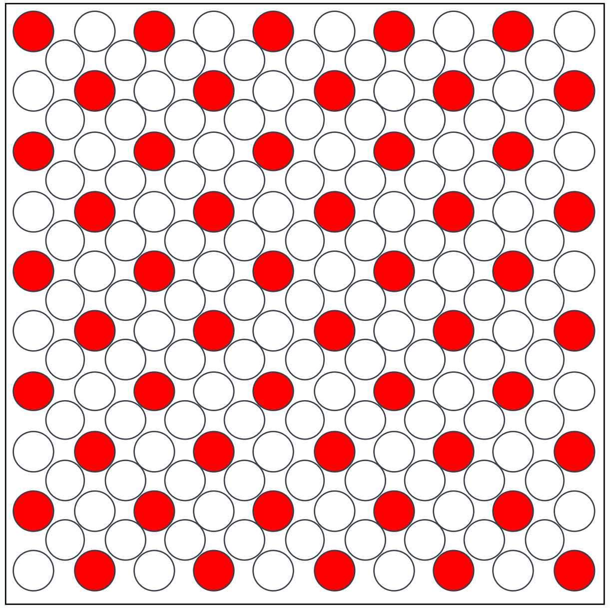
Random



Entropically driven

???

Ordered



Enthalpically driven

Models of Short range order

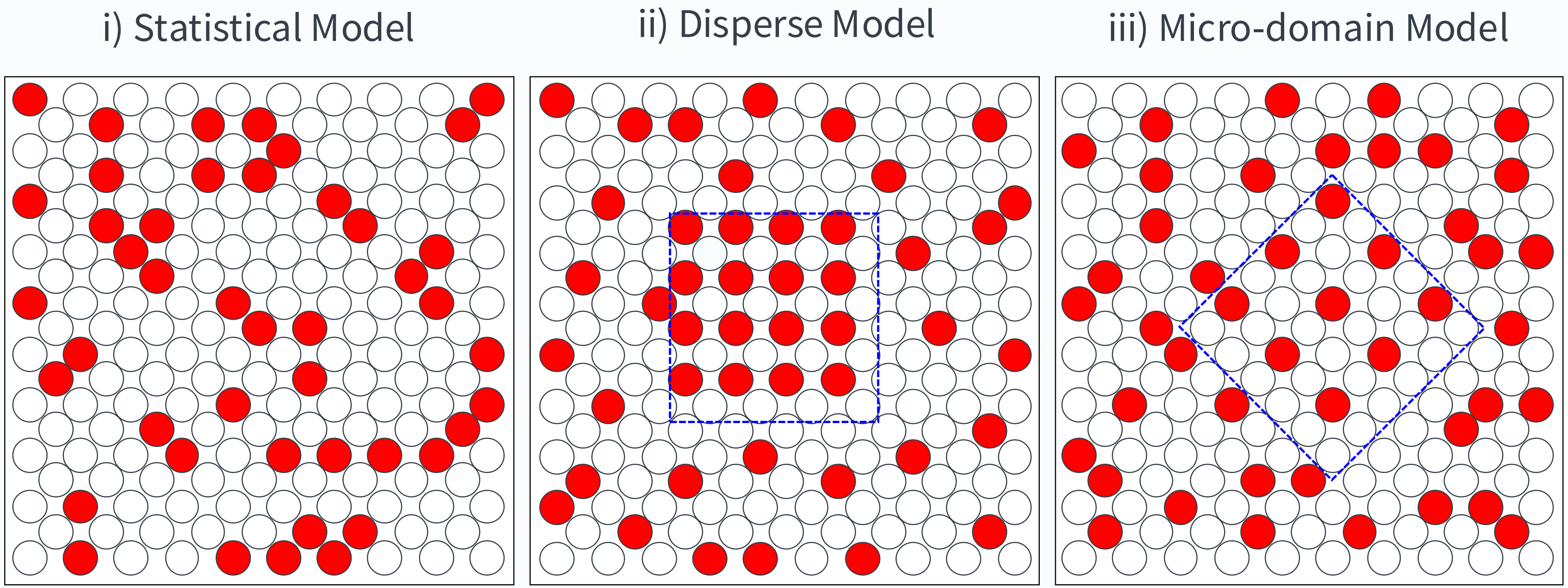


Fig. 6 – Models of the different types of short range order (SRO) that can occur in a system. From left to right they are the statistical model, the disperse model and the micro-domain model. The blue boxes indicate the small regions of LRO in the system. All the models are 25% red atoms, 75% white.

"A New Approach to the Analysis of Short-range Order in Alloys using total scattering" - L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, Acta Materialia, 115 (2016) 155-166

Original studies of local structure in alloys

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PHYSICAL REVIEW VOLUME 77, NUMBER 5 MARCH 1, 1950

An Approximate Theory of Order in Alloys*,**

J. M. COWLEY***
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received October 26, 1949)

Short-range order parameters α_i are defined to express the interaction of a given atom in an alloy with the atoms of the ith shell of atoms surrounding it. From simple thermodynamic reasoning, involving a certain degree of approximation, equations relating the α_i with energy terms and the temperature are derived. Equations for the long-range order parameter, S, are obtained by considering the limiting case of i very large. The values of the long- and short-range order parameters obtained by solving these equations

Zeitschrift für Physik, Bd. 129, S. 219—232 (1951).

Über Widerstandslegierungen*.

Von
HANS THOMAS, Hanau.
(Mitteilung aus dem Laboratorium der Vacuumschmelze AG.)

Mit 15 Figuren im Text.

(Eingegangen am 16. Dezember 1950.)

Eine Reihe von Legierungen, die aus primären Mischkristallen bestehen und wenigstens ein Übergangsmetall als Komponente enthalten, zeigt als Besonderheiten, daß die Widerstand-Temperaturkurve S-förmig gekrümmt ist und daß der Widerstand im weichen und im harten Zustand durch Wärmebehandlung bei niedrigen Temperaturen ansteigt und durch Kaltverformung erniedrigt wird. Dieses Verhalten läßt sich darauf zurückführen, daß sich bei niedrigen Temperaturen ein ganz bestimmter Zustand ausbildet, der sich durch erhöhten elektrischen Wider-

Überstruktur und K-Zustand im System Nickel-Chrom*)**)

Von Hans Günter Baer in Hanau a.M.
(Aus dem Laboratorium der Vacuumschmelze AG., Hanau)

Versuchsdurchführung — Röntgenographischer Nachweis der Ordnungsphase Ni_2Cr — Existenzgebiet von Ni_2Cr und Bildungskinetik — Neubestimmung der Löslichkeitslinie für Chrom in Nickel — Folgerungen

Die homogenen Mischkristalle mancher Metalle, z. B. Nickel mit Chrom, Molybdän oder Aluminium, Eisen mit Aluminium, Kupfer mit Nickel, oder ternäre Legierungen, wie Nickel-Chrom-Eisen, Eisen-Aluminium-Chrom oder Kupfer-Nickel-Zink, zeigen Anomalien in ihren physikalischen Eigenschaften, für deren Charakterisierung sich nach dem Vorschlag von H. Thomas[1]) der Begriff K-Zustand eingebürgert hat. Nach der von ihm stammenden ausführlichen

gung bei einer Legierung, die 28 At.-% Cr enthielt und die nach einer Vorglühung längere Zeit in der Gegend von 500° getempert worden war, eine Nahordnung nachzuweisen. Sie kommen zu dem Schluß, daß ein hoher Grad von Nahordnung nicht vorhanden sein kann.

Die Verknüpfung des K-Zustandes mit einer Änderung des Auffüllungsgrades der inneren Elektronenschalen im Sinne eines Elektronenrücktritts allein

Consequences

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- Strengthening – variation in dislocation motion due to ordering and lattice distortion effects combined
- Electrical resistivity
- Magnetic properties
- Thermodynamic discontinuities
- Corrosion resistance
- Radiation damage

3rd World Congress in High Entropy Alloys

Mosaic

3rd World Congress in High Entropy Alloys

9:05 AM Invited
Short Range Order and the Evolution ... in the CrCoNi Medium Entropy Alloy
California-Berkeley
This talk will describ... and nanomechani... multiscale deform... alloy. In order to u... terms of the evol... of 4D-STEM wa... experiments. 4D... diffraction anal... perform strain... situ deformati... then correlate... to examine h... Lastly, we wi... both the m... via electron... MEA.

9:35 AM
Understa... Order in...

11:15 AM
Diffuse Electron Scattering Reveals Kinetic Frustration as Origin ... Order in CoCrNi Medium Entropy Alloy: *Annie Barnett*[1]; ... Mitra Taheri[1]; Michael Falk[1]; [1]Johns Hopkins Uni...
Equimolar CoCrNi is driven towards a lon... ...ation characteristics similar to tha... ...try and applied

2:55 PM
Quantitative Assessment of Local Chemical Ordering in Atomistic Simulations of High-entropy Alloys: *Killian Sheriff*[1]; Yifan Cao[1]; Rodrigo Freitas[1]; [1]Massachusetts Institute of Technology
High-entropy alloys (HEAs) exhibit exceptionally good combinations of properties recently reported to correlate with chemical short-range ordering (cSRO). However, in atomistic simulations, their state of cSRO has only been so far characterized using the Warren-Cowley parameters. Yet, this approach is incomplete as distinct local atomic configurations sharing the same chemical concentration are indistinguishable. Here, we propose a generalized framework, based on graph-convolution neural networks equivariant to E(3) symmetry operations, statistical mechanics, and information theory, capable of completely identifying the set of distinct local atomic bonding environments and their associated population densities in HEAs. This approach leads to a quantitative characterization of the cSRO state and provides a predictive framework for evaluation of cSRO domain sizes, thus offering novel avenues to explore the relationships between processing, structure, and properties in HEAs.

3:15 PM Break

3:35 PM
Capturing Short-range Order in High-entropy Alloys with Machine-learning Potentials: *Yifan Cao*[1]; Killian Sheriff[1]; Rodrigo Freitas[1]; [1]Massachusetts Institute of Technology
Chemical short-range order (cSRO) is recently reported to strongly influence the mechanical properties of various high-entropy alloys (HEA). However, the intricate nature of cSRO has made it challenging for current machine-learning potentials (MLP) to capture this feature, and many proposed approaches lack quanti... of MLP performance on this ta... generalized ...

4:55 PM
Atomic Representations of Local and Global Chemical Effects of Mechanical Strength: *Mitchell Wood*[1]; Megan McCarthy[1]; Mary Alice Cusentino[1]; [1]Sandia National Laboratories
...exceptional properties observed in complex concentrated ...As) arise from the interplay between crystalline order ...ical disorder at the atomic scale, complicating the ...ation of properties. The base metallurgical argument ...s' observed strength is the maximization of solid solution ...thening effects, but is difficult to quantitatively address ...experiments alone. Herein we present a quantum-accurate ...ratomic potential (IAP) for use in molecular dynamics simulations MoNbTaTi that efficiently scales to systems that are converged ...ith respect to size, time and chemical complexity. Furthermore, we use this IAP to quantify the relationship between inhomogeneous lattice strains and novel definitions of local chemical environment. We will highlight the improvement of this reduced order model over historical arguments of local atomic volume and element-wise attribution of strengthening in these complex alloys.

...55 AM
...wards More Robust EXAFS Analysis for Quantifying Short Range ...der in Multicomponent Alloys: *Brian DeCost*[1]; Bruce Ravel[1]; ... McQueen[2]; Mitra Taheri[2]; Howie Joress[1]; [1]National Institute of ...ards and Technology; [2]Johns Hopkins University
...research has found that chemical short range order in high ...alloys (HEAs) can play an important role on properties ...mechanical strength and corrosion resistance. EXAFS is ...g measurement technique for quantifying this aspect ...y structure and chemistry; however, the complexity of ...required for realistic analysis of multicomponent HEA ...s a substantial barrier to obtaining meaningful insight. ...rincipled Bayesian data analysis approach to EXAFS ...ove its reliability. We also show a novel approach to ...ical constraints into EXAFS models, with a focusing ...etween the short range order parameters ...s in solid solutions. Our long term goal is ...sis that can drive adaptive measure... enabling comprehensive under... composition and short r...

...insights from ... ...ius Bacurau[1]; Angelo ... Field[2]; Michael Kaufman[2]; ...ão Carlos; [2]Colorado School of Mines
...uss the challenges of characterizing short-range ...lti-Principal Element Alloys (MPEAs), especially in ...bic (FCC) alloys. A series of results using direct and ... for characterizing SRO in CrCoNi and FeC... ...and compared. The indirect method... ...onal properties. The ...

...atom Approach for Simulating Refractory ...: *Chloe Zeller*[1]; Ellad Tadmor[1]; [1]University of ...
...y alloys (RHEAs) are characterized by their high ...and superior strength and are thus promising ...nvironment aerospace applications, such as ...thermal protection materials on hypersonic ...molecular dynamics (MD) simulations are a ...or predicting the thermomechanical response ...rge simulations are required to obtain good ...for local chemical fluctuations that can have ...erties. To reduce system size ...

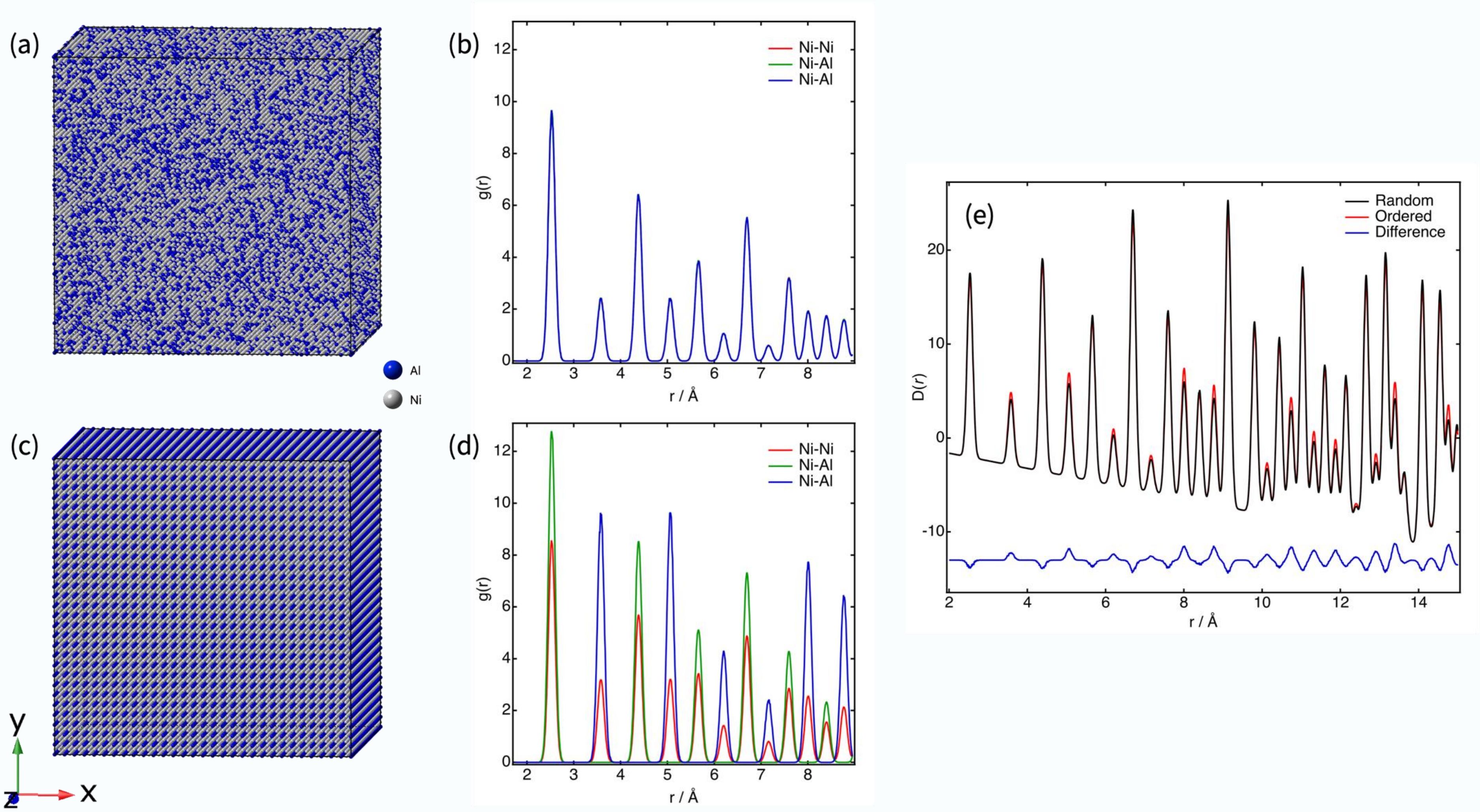
1:45 PM Invited
Quantifying Short-range Order and its Domain Size in High-entropy Alloys: *Rodrigo Freitas*[1]; [1]Massachusetts Institute of Technology
Complete characterization of short-range order is challenging to realize because of the sheer number of local chemical configurations that must be accounted for. Moreover, the chemical complexity of concentrated solid-solution phases is often described as the tendency for some of these configurations to be more common than others (i.e., "slightly less random than completely random"), which does not translate easily into a physically intuitive and quantifiable picture. In this talk I will introduce an approach that combines statistical mechanics and information theory with machine learning techniques to quantify the space of local chemical configurations available for high-entropy alloys. I will show that this a... ...predictive framework for evaluation of short-ran...

Chapter 2

Applying total scattering to metallurgical systems

What affect does the ordering have on the PDF?

Mosaic



Mosaic

Acta Materialia 115 (2016) 155–166

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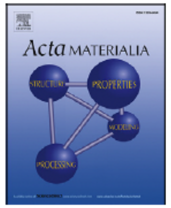

Full length article

A new approach to the analysis of short-range order in alloys using total scattering

L.R. Owen [a, b], H.Y. Playford [b, *], H.J. Stone [a], M.G. Tucker [b, c, 1]

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[b] ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, UK
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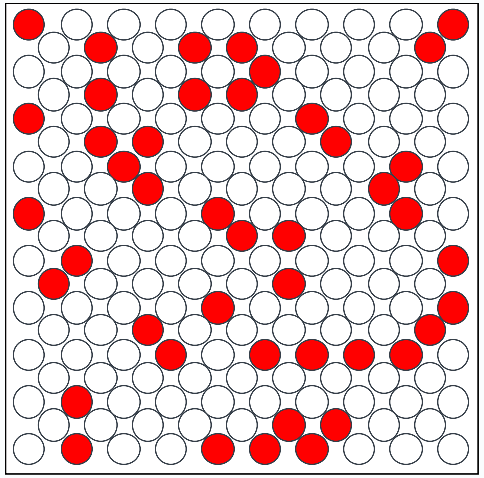
ABSTRACT

In spite of its influence on a number of physical properties, short-range order in crystalline alloys has received little recent attention, largely due to the complexity of the experimental methods involved. In this work, a novel approach that could be used for the analysis of ordering transitions and short-range order in crystalline alloys using total scattering and reverse Monte Carlo (RMC) refinements is presented. Calculated pair distribution functions representative of different types of short-range order are used to illustrate the level of information contained within these experimentally accessible functions and the insight into ordering which may be obtained using this new method. Key considerations in the acquisition of data of sufficient quality for successful analysis are also discussed. It is shown that the atomistic models obtained from RMC refinements may be analysed to identify directly the Clapp configurations that are present. It is further shown how these configurations can be enhanced compared with a random structure, and how their degradation pathways and the distribution of Warren-Cowley parameters, can then be used to obtain a detailed, quantitative structural description of the short-range order occurring in crystalline alloys.

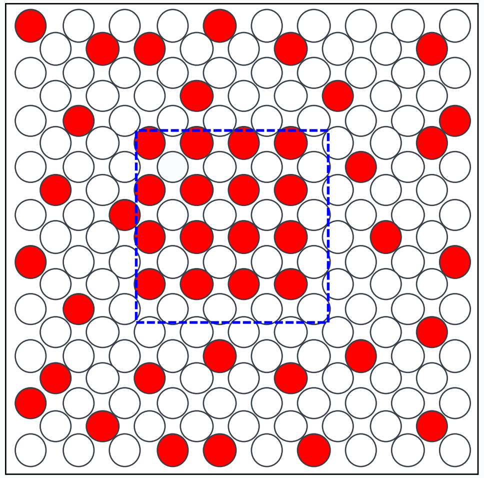
Models of Short range order

Mosaic

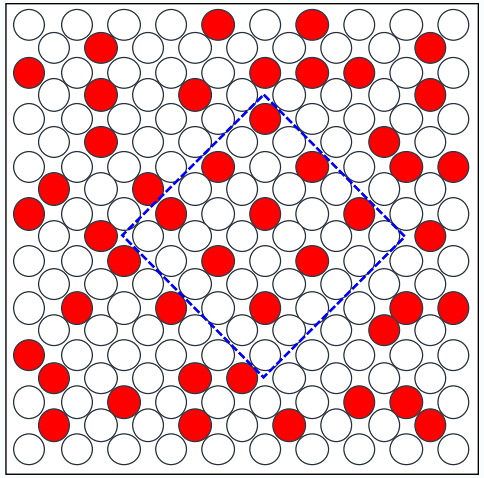
Statistical

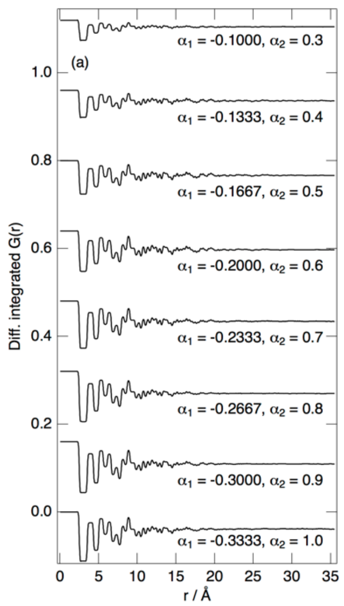


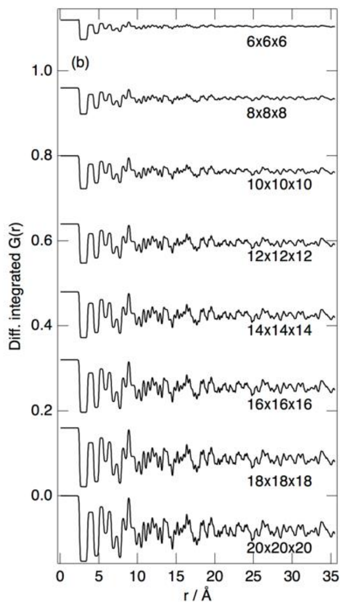
Disperse

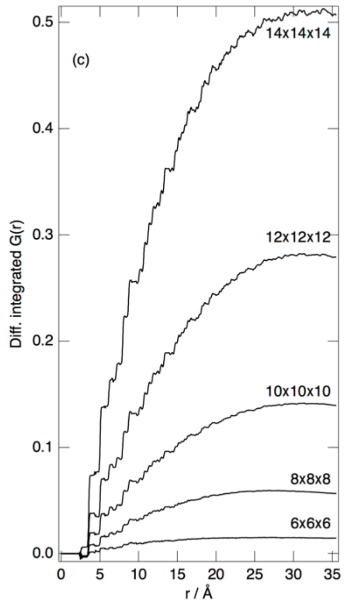


Micro-domain

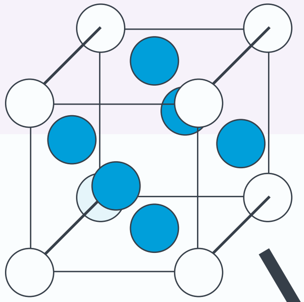


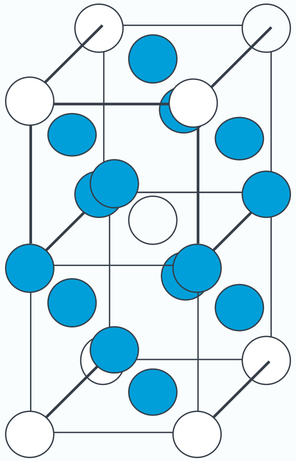


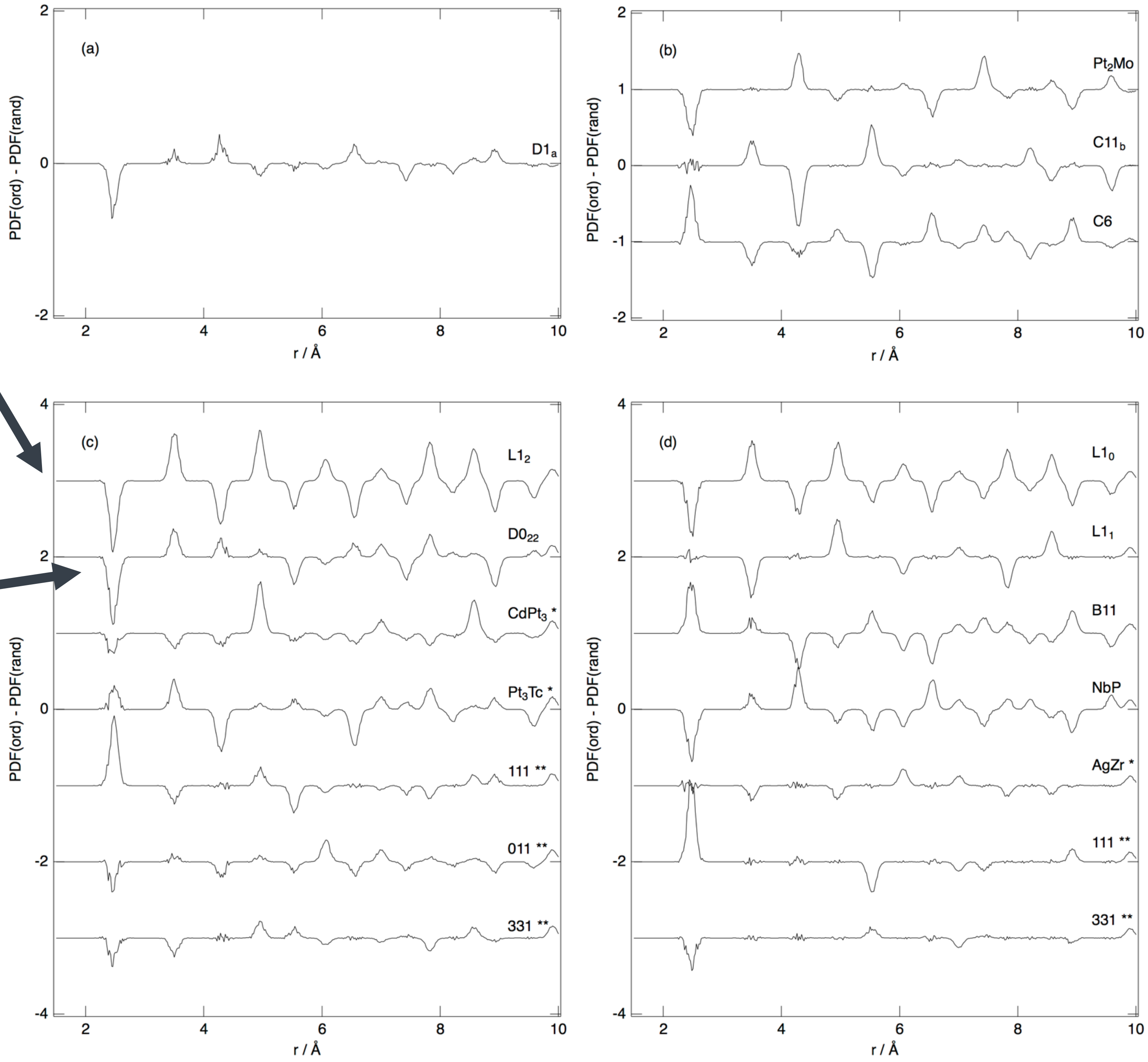


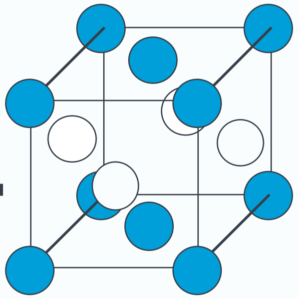


"A New Approach to the Analysis of Short-range Order in Alloys using total scattering" - L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, Acta Materialia, 115 (2016) 155-166









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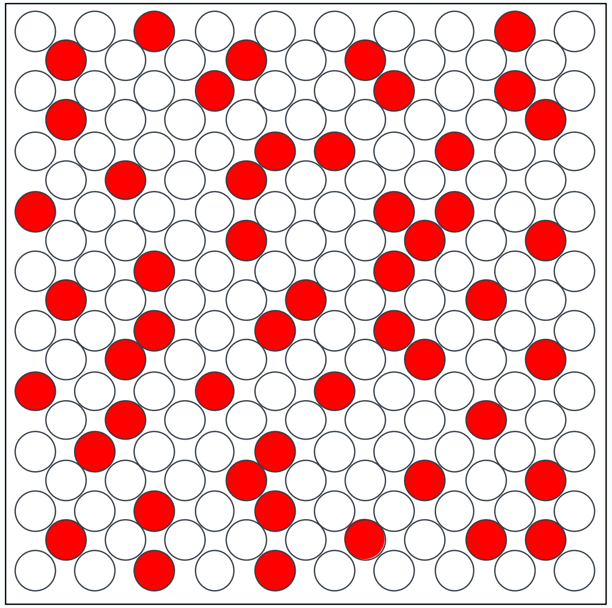
2. Quantification

Ordered and Random structures

Mosaic

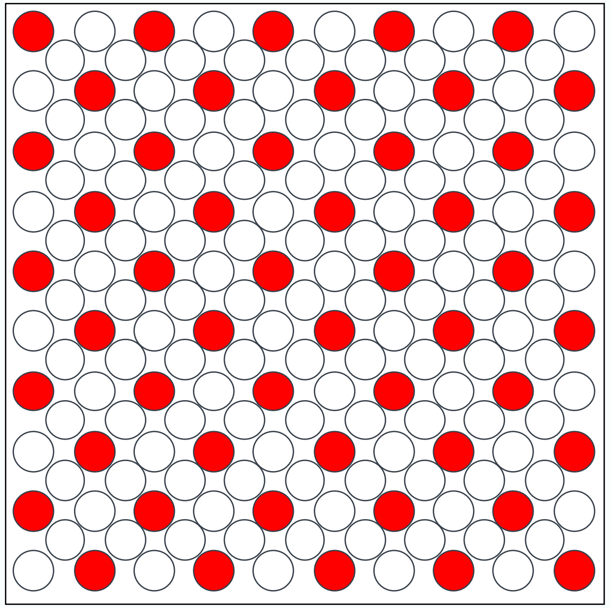
Random



Entropically driven

???

Ordered



Enthalpically driven

SRO in alloys – Warren-Cowley parameters

Mosaic

We define:

$$\alpha_{lmn} = 1 - \frac{P_{lmn}^{AB}}{c^{B}} = 1 - \frac{P_{lmn}^{BA}}{c^{A}}$$

Where c is a concentration of a particular atom type in the alloy and P^{BA} the probability of finding an A atom (second letter in superscript) at *lmn* from a B atom (and vice-versa).

Random $\alpha = 0$

All like atoms $\alpha = 1$

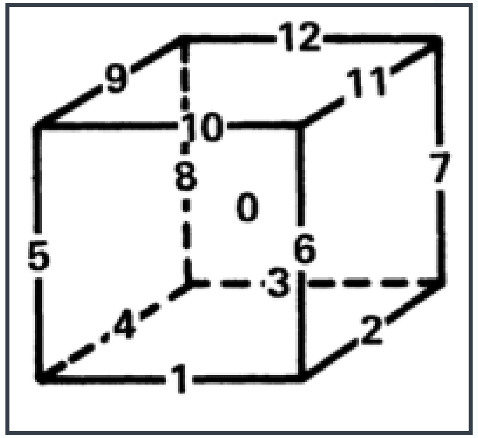
All dislike atoms $\alpha = 1- (1/c)$

Clapp configurations

Mosaic

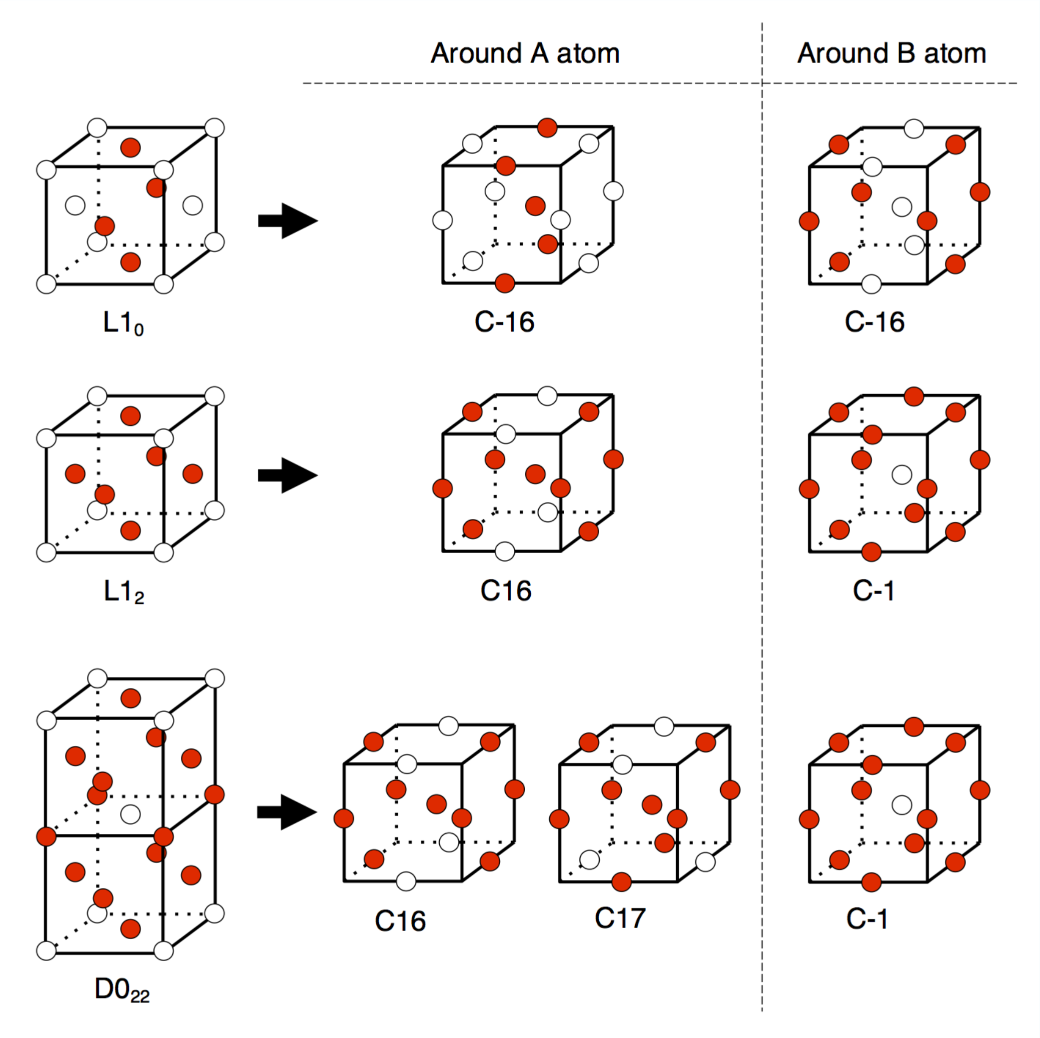
TABLE XIII. PVM parameters for fcc nearest-neighbor cluster. See Fig. 4 for site indices.

Index k	Sites with $\sigma_i = -1$	Multiplicity W_k	Composition $W_k \langle\sigma\rangle_k$	First neighbor $W_k C_k^1$	Second neighbor $W_k C_k^2$	Third neighbor $W_k C_k^3$	Fourth neighbor $W_k C_k^4$
1($\bar{1}$)	···	1	+1(−1)	+1	+1	+1	+1
2($\bar{2}$)	6	12	+10(−10)	+8	+8	+8	+8
3($\bar{3}$)	6,7	12	+8(−8)	+4	+8	+4	+4
4($\bar{4}$)	5,7	6	+4(−4)	+2	+2	+2	+6
5($\bar{5}$)	6,12	24	+16(−16)	+8	+8	+12	+8
6($\bar{6}$)	6,11	24	+16(−16)	+12	+8	+8	+8
7($\bar{7}$)	5,6,7	12	+6(−6)	0	+8	0	+8
8($\bar{8}$)	5,6,12	24	+12(−12)	0	+8	+8	0
9($\bar{9}$)	1,7,9	8	+4(−4)	0	0	+4	0
10($\overline{10}$)	5,6,11	48	+24(−24)	+8	+16	+8	0
11($\overline{11}$)	4,6,11	48	+24(−24)	+8	0		
12($\overline{12}$)	1,5,11	24	+12(−12)	+4	0		
13($\overline{13}$)	2,6,11	24	+12(−12)	+8	+8		
14($\overline{14}$)	1,6,11	24	+12(−12)	+8	0		
15($\overline{15}$)	6,10,11	8	+4(−4)	+4	0		
16($\overline{16}$)	5,6,7,8	3	+1(−1)	−1	+3		
17($\overline{17}$)	4,6,7,9	6	+2(−2)	−2	+2		
18($\overline{18}$)	5,6,8,11	48	+16(−16)	−8	+16		
19($\overline{19}$)	3,5,6,11	48	+16(−16)	−8	0		
20($\overline{20}$)	1,5,10,12	48	+16(−16)	0	+16		
21($\overline{21}$)	1,6,7,10	24	+8(−8)	0	+8		
22($\overline{22}$)	5,6,9,11	12	+4(−4)	0	+4		



“Atomic Configurations in Binary Alloys” – P.C. Clapp, *Physical Review B*, 4, 2 (1971), 255-270.

Clapp configurations for some standard LRO structures



"A New Approach to the Analysis of Short-range Order in Alloys using total scattering" - L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, Acta Materialia, 115 (2016) 155-166

Clapp configuration - Enhancement factors

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$$p_a = m_a[x^n(1-x)^{13-n} + x^{13-n}(1-x)^n]$$

$$\overline{n_a} = p_a N$$

$$\sigma_a = \sqrt{p_a(1-p_a)N}$$

$$\beta_a = \frac{(n_a - \overline{n_a})}{\sigma_a}$$

p_a is the probability of configuration a being occupied, m_a the multiplicity of that configuration, x the concentration of species A, n the number of atoms of type a in the 12 nearest neighbours of the configuration, N the total number of atoms, and n_a and variants therefore the number of atoms in that configuration.

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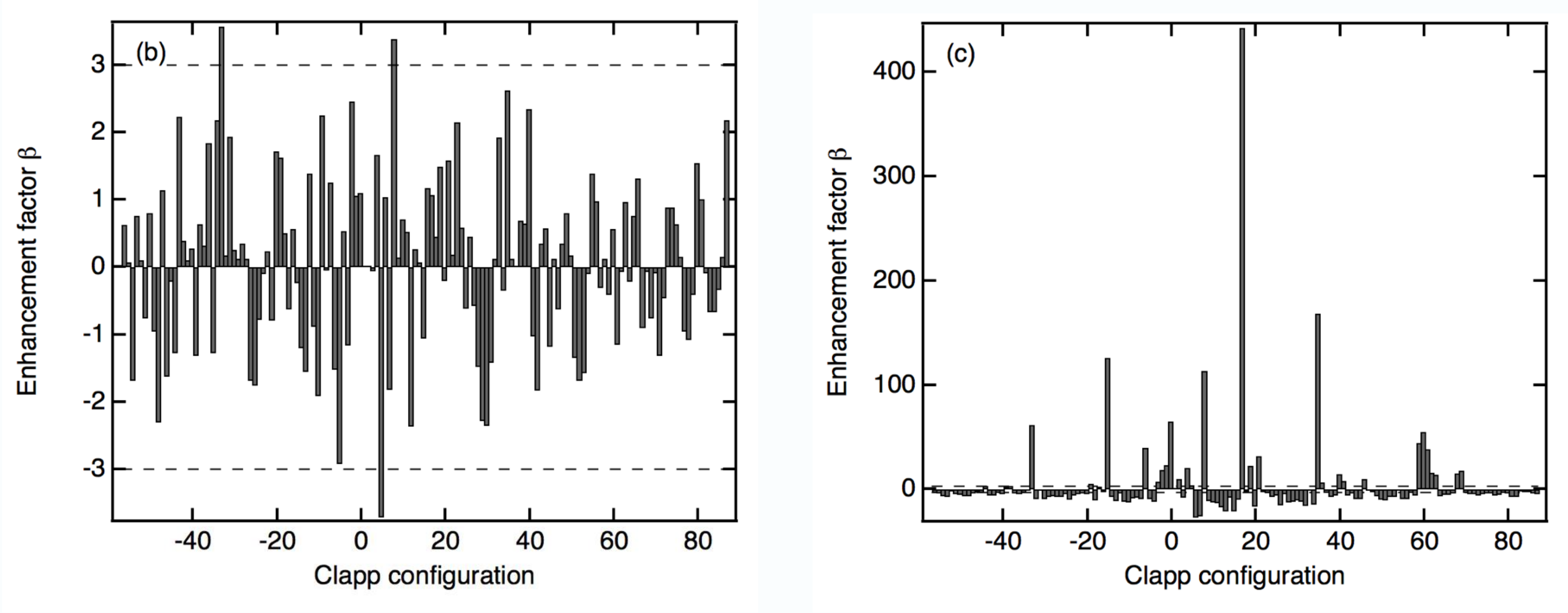
Enhancement factors



3. Demonstration

Acta Materialia 125 (2017) 15–26

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Full length article

Analysis of short-range order in Cu_3Au using X-ray pair distribution functions

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[b] ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire, OX11 0QX, UK
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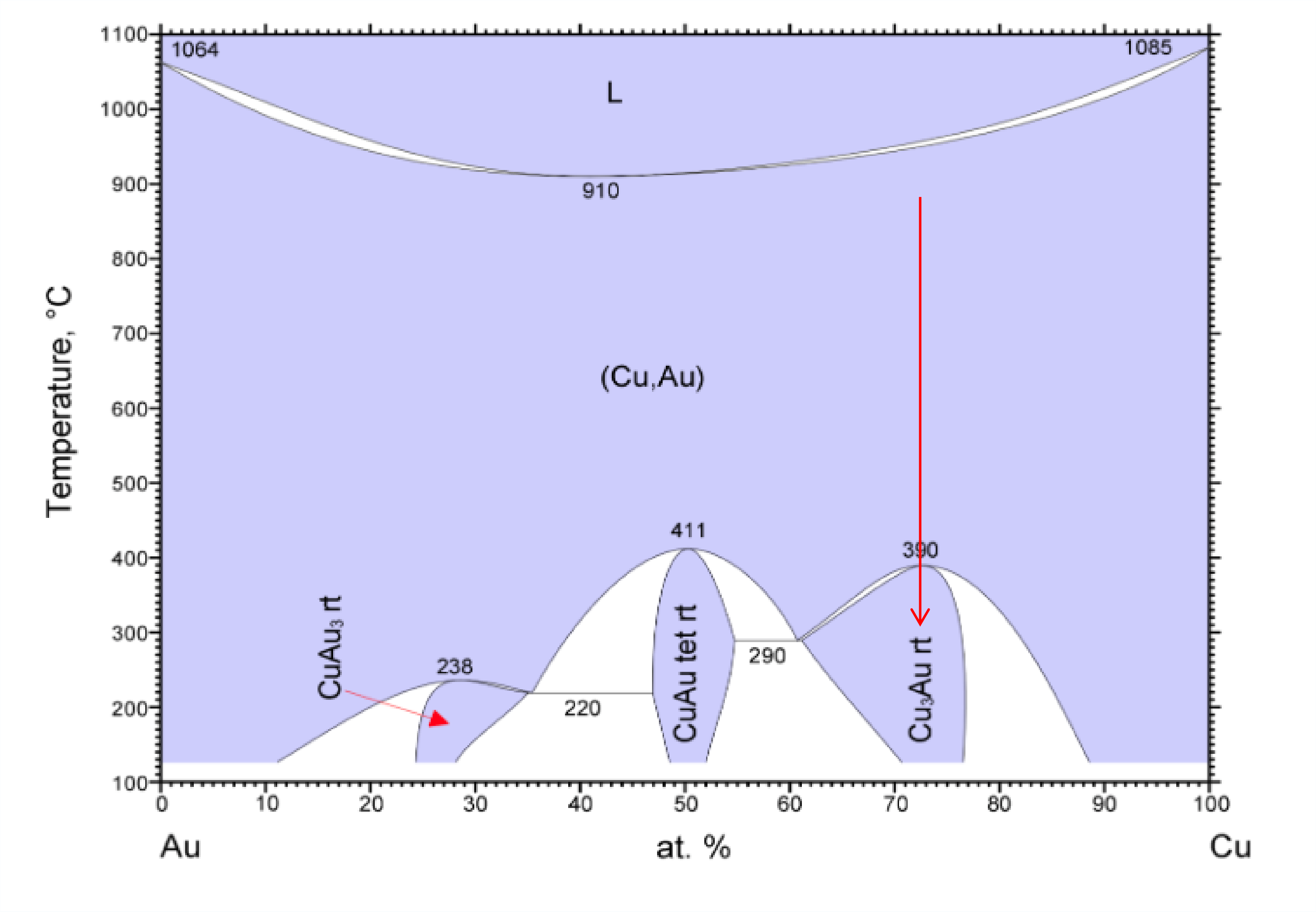
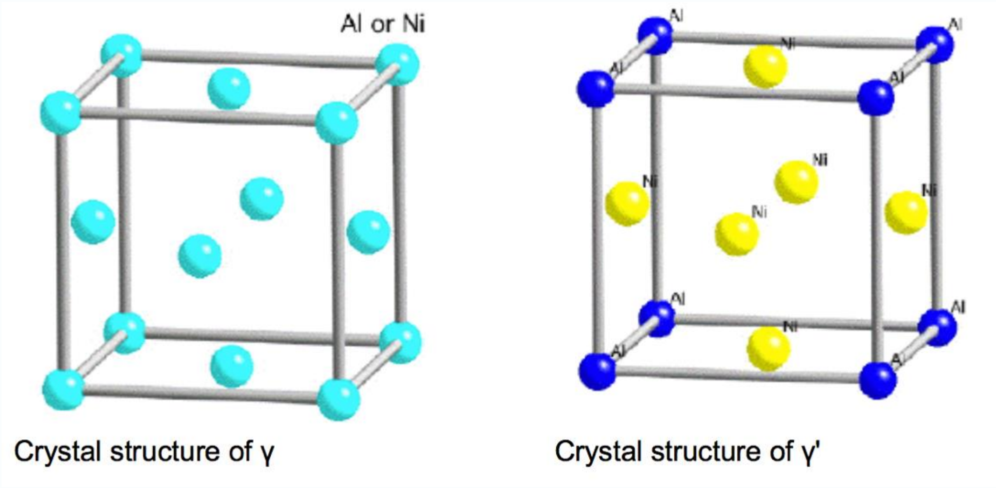
A B S T R A C T

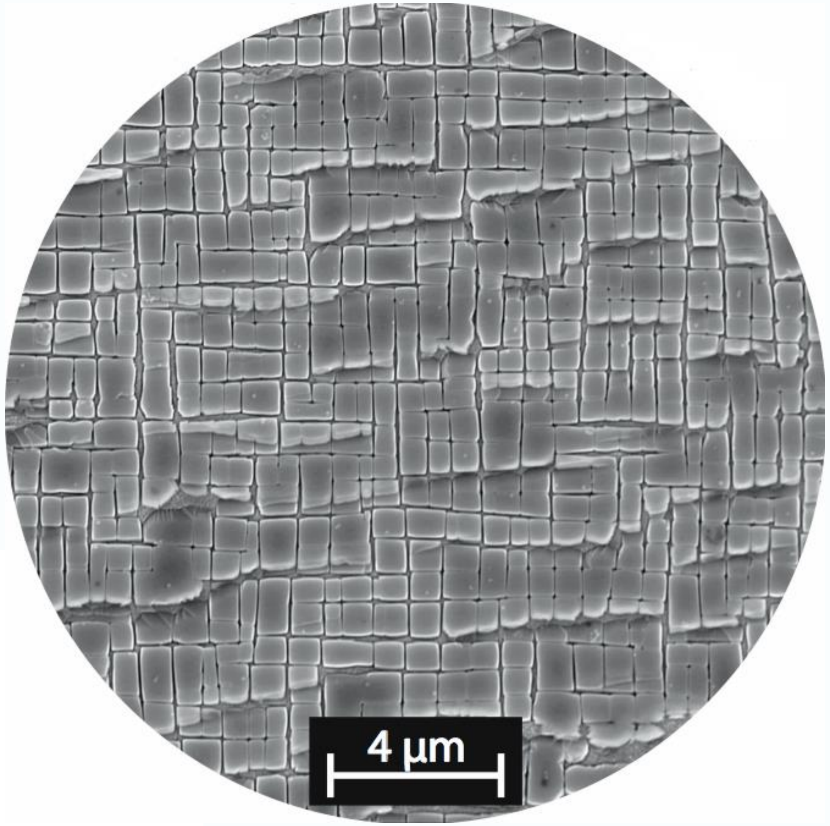
Cu_3Au is often cited as a case example of a metallic system exhibiting both short-range order in the solid solution phase and a long-range order-disorder transition. In this work, X-ray total scattering data obtained from the *in situ* heating of a gas-atomised powder sample of Cu_3Au are used to demonstrate the suitability of total scattering, in conjunction with large-box modelling, for the analysis of short-range order in alloys. The existence of an ordering transition at c. 400° is confirmed, and the development of short-range order reminiscent of the $L1_2$ long-range ordered structure is observed prior to this transition. Furthermore, it is found that a degree of short-range order is present even in quenched samples (usually assumed to be completely random) which throws into question the identification of short-range order in previous ex situ studies. It is demonstrated that total scattering can be used successfully to identify the type and degree of ordering, differences in the bond length distributions in the first coordination shell and to suggest a likely mechanism for the formation of order in the system.

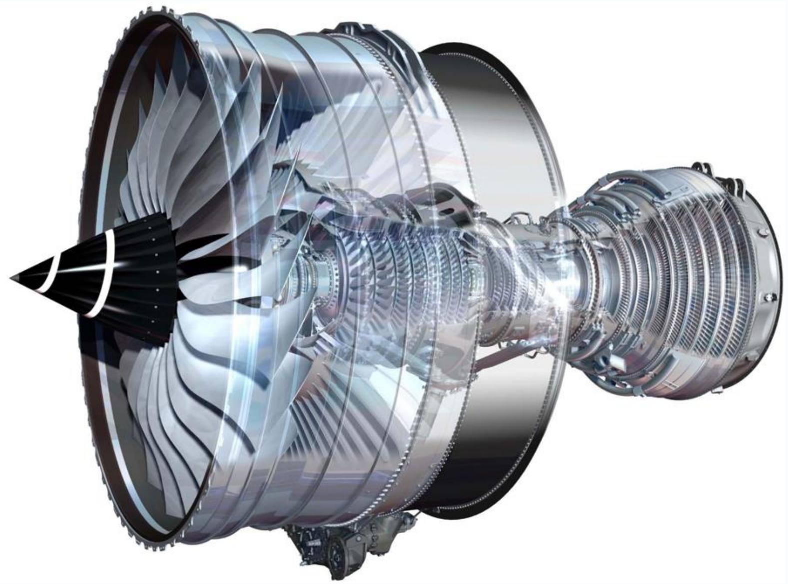
Cu_3Au – On cooling

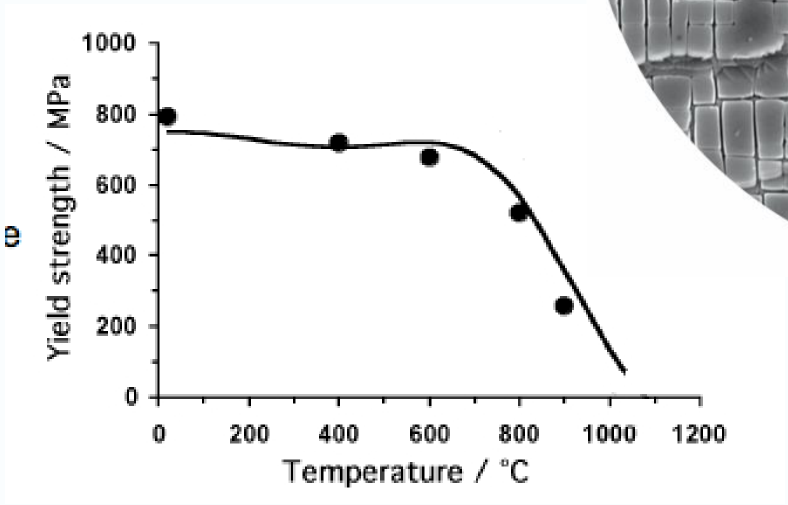


Nickel Superalloys

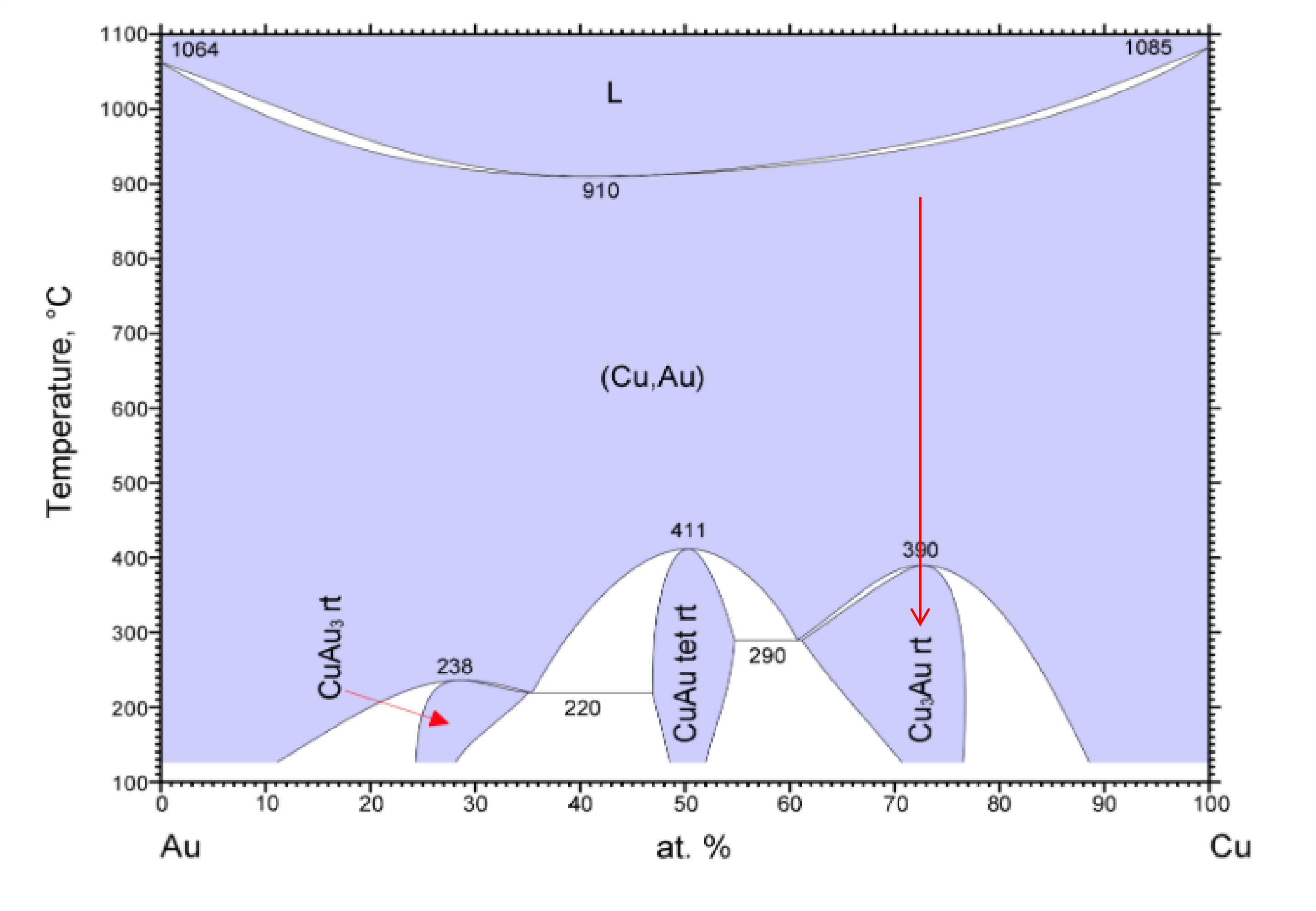








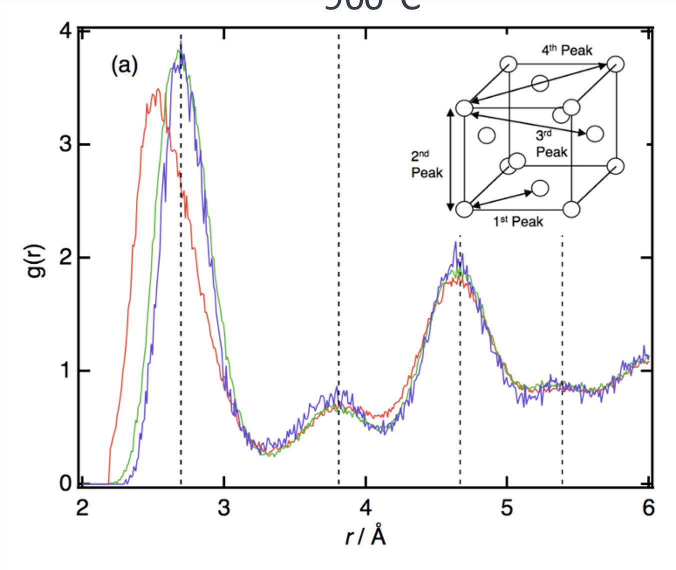
Cu_3Au – On cooling



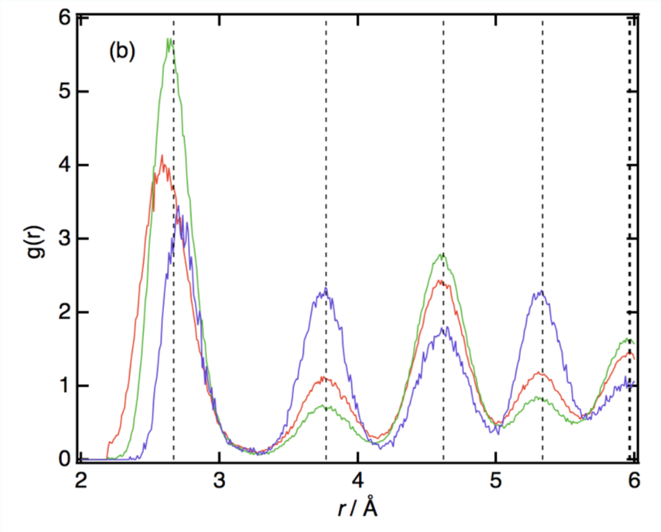
Analysis

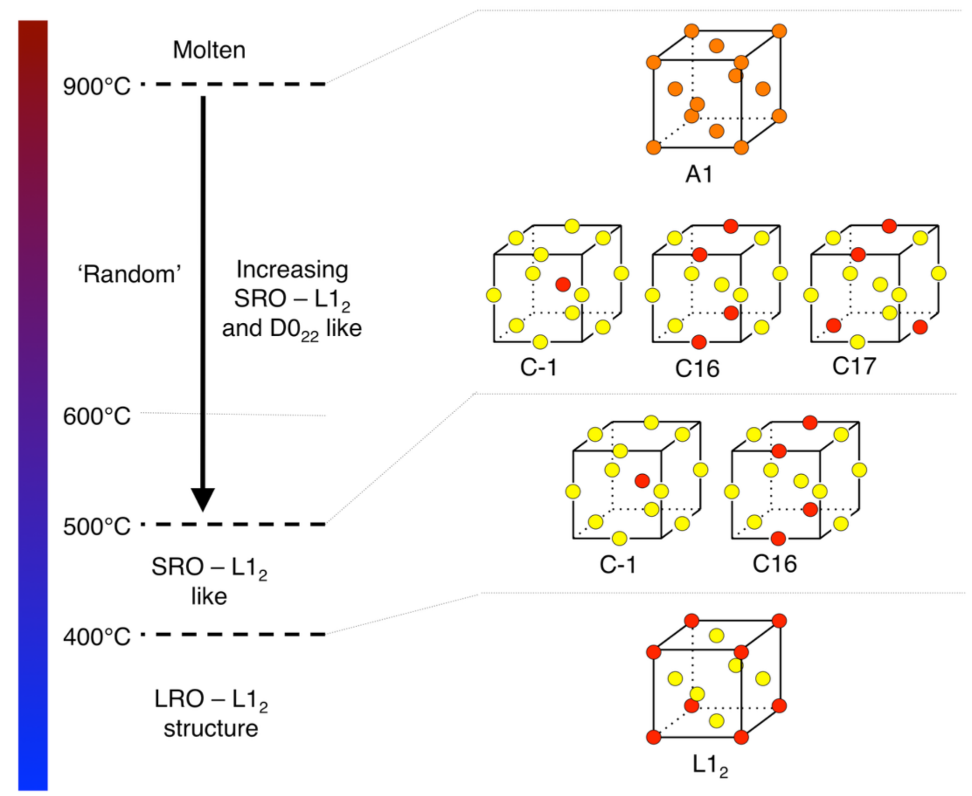
Mosaic

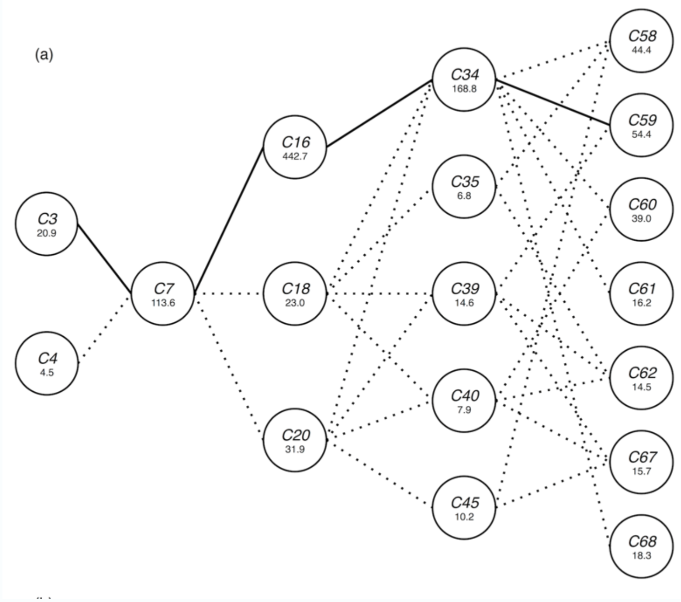
900°C

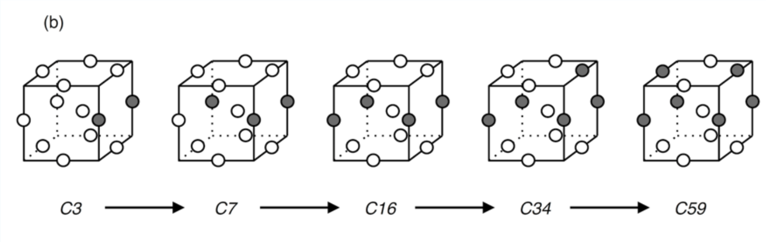


400°C









L.R. Owen, H.Y. Playford, H.J. Stone and M.G. Tucker "Analysis of Short-Range Order in Cu_3Au using X-ray Pair Distribution Functions", *Acta Materialia,* 125 (2017) 15-26.

Challenges

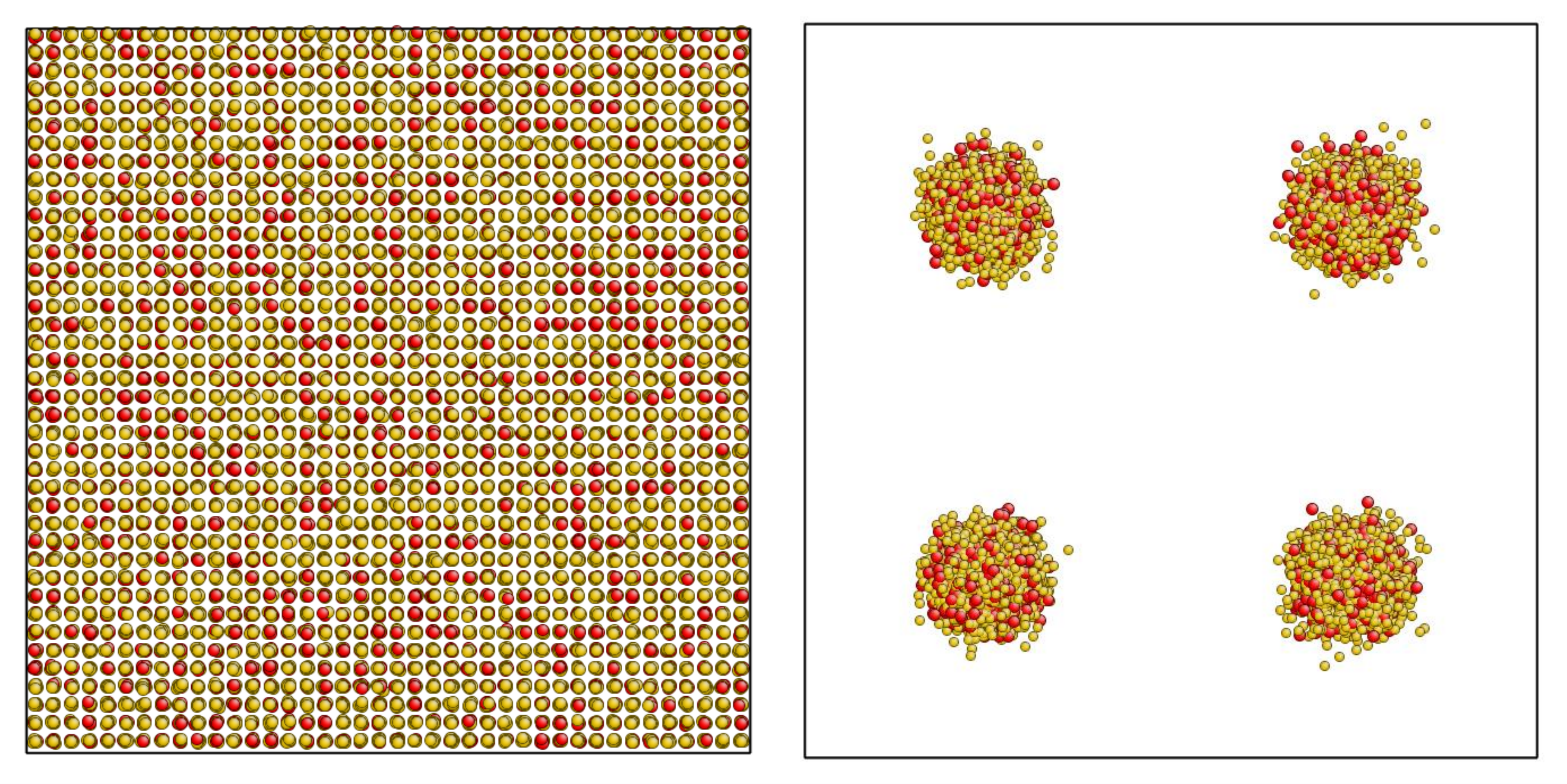
Some possible errors

Mosaic

- Incorrect lattice parameter
- Offset in the data
- Instrumental resolution function
- Incorrect scaling
- Texture

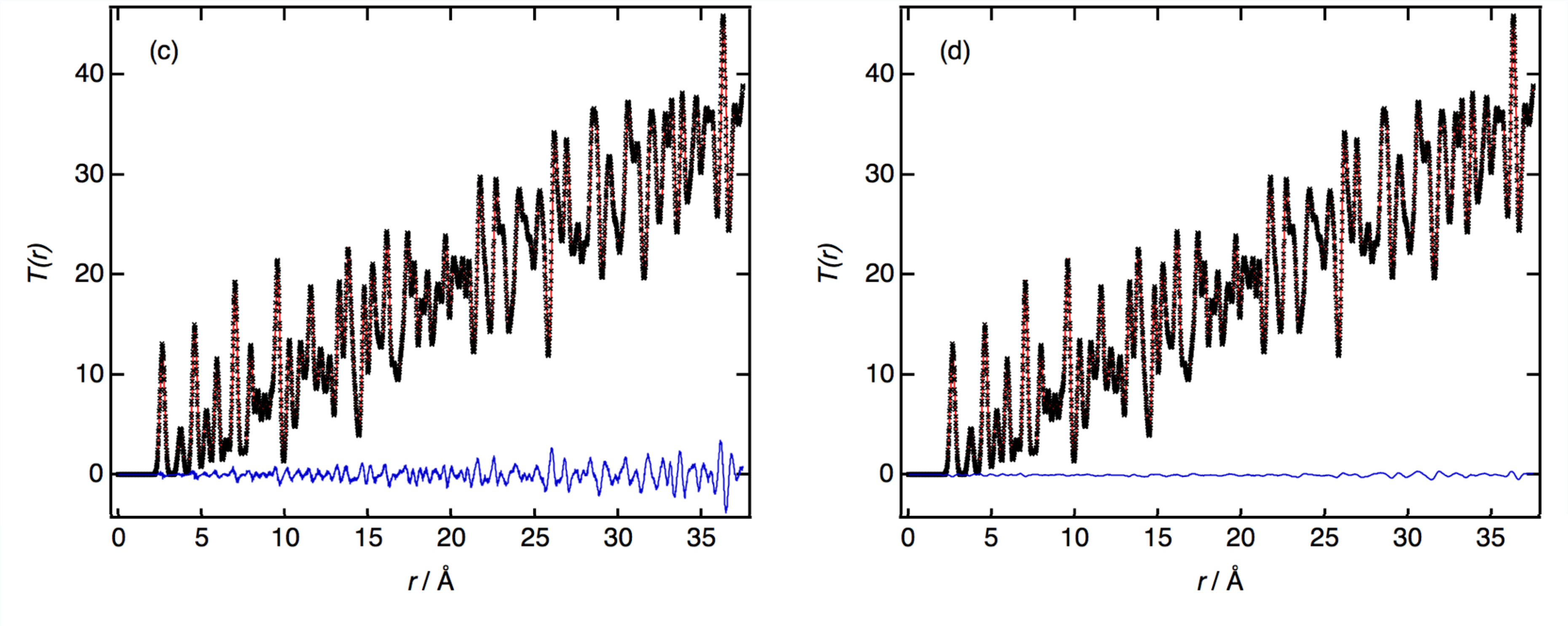
Fit to simulated data

Mosaic



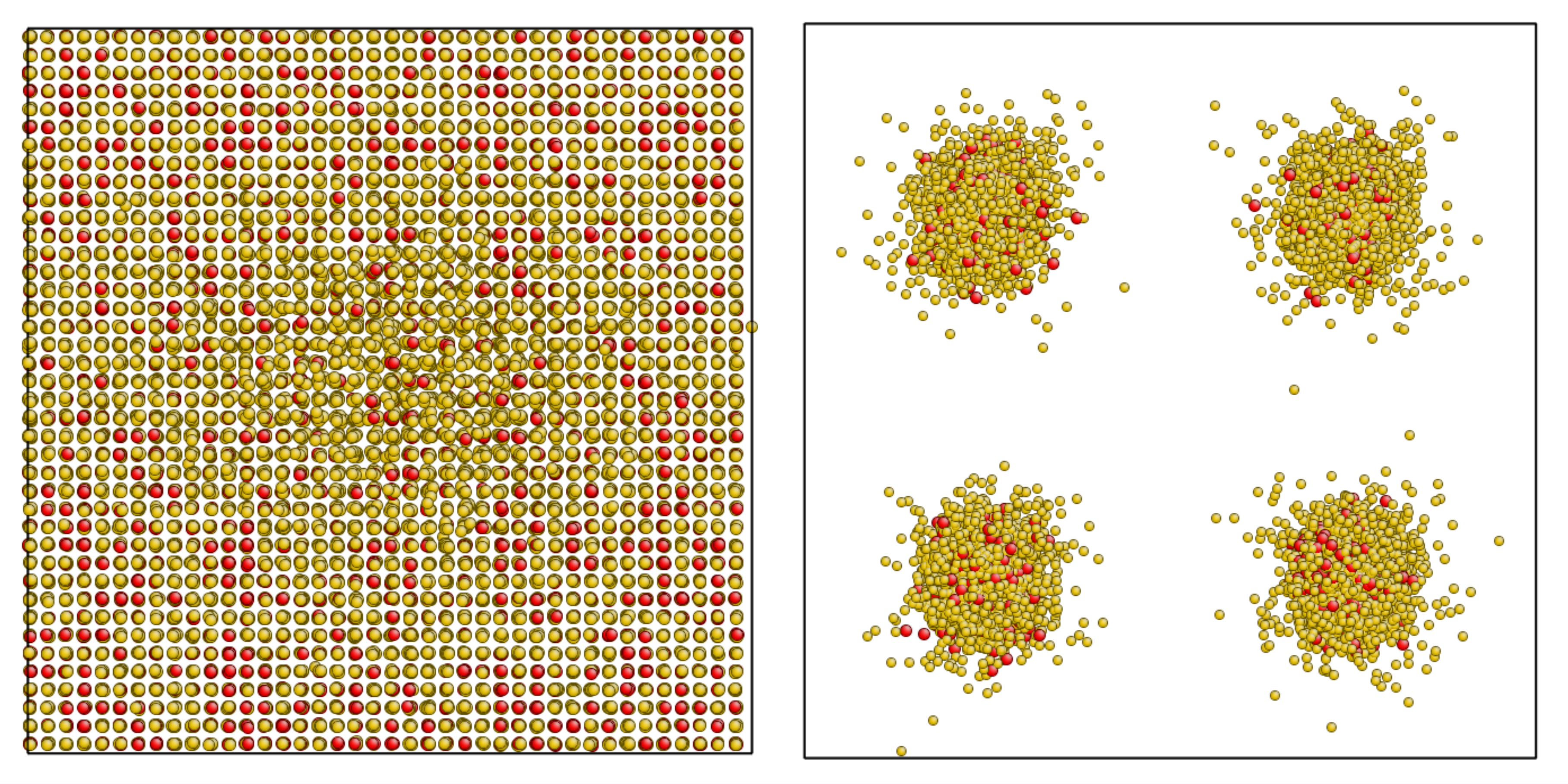
L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, *Acta Materialia,* 125 (2017) 15-26

Incorrect lattice parameter



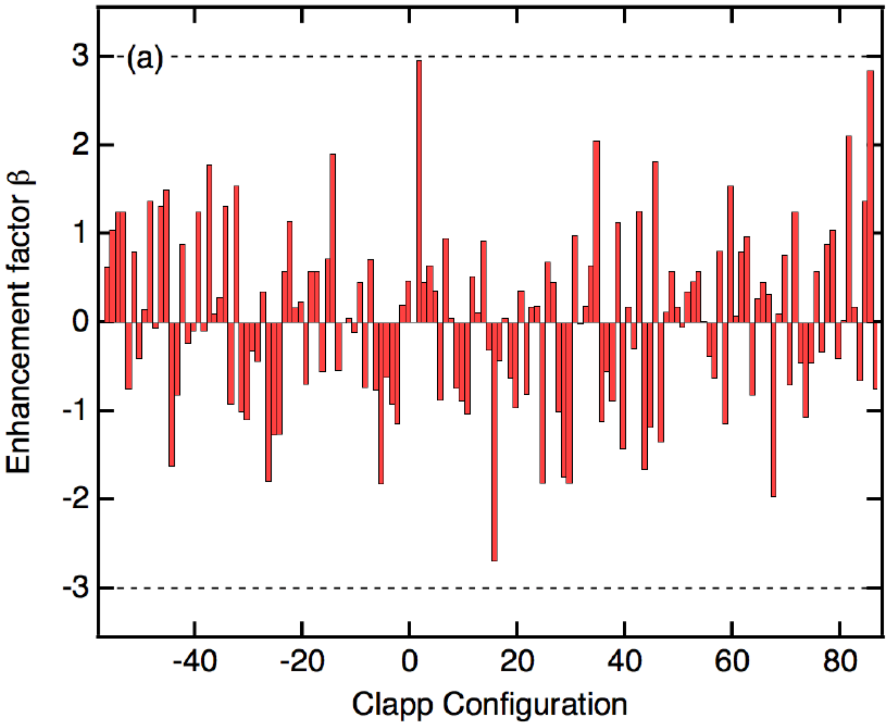
L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, *Acta Materialia,* 125 (2017) 15-26

Incorrect lattice parameter

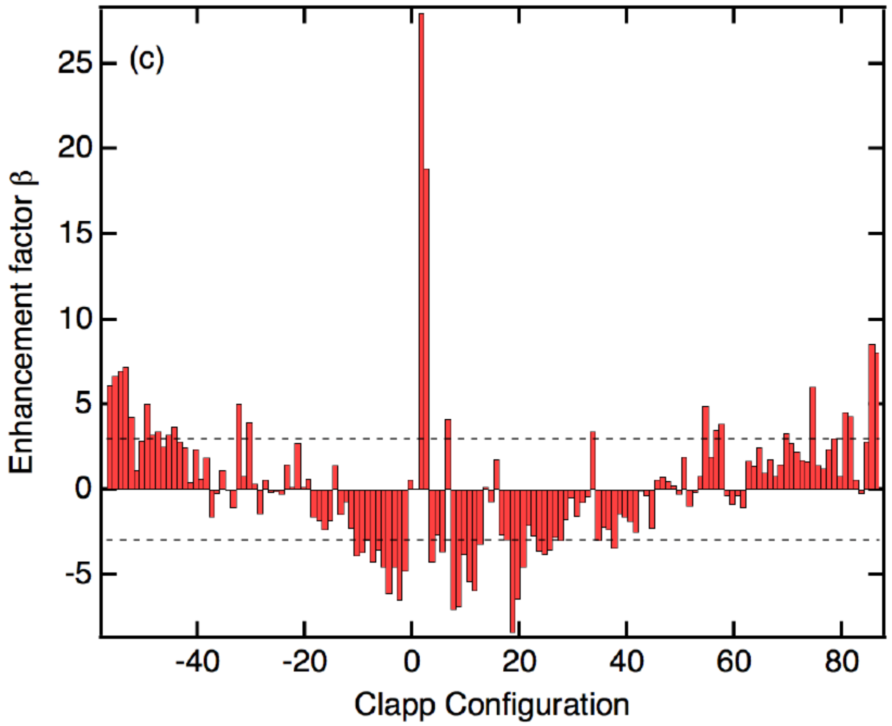


L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, *Acta Materialia,* 125 (2017) 15-26

Incorrect lattice parameter



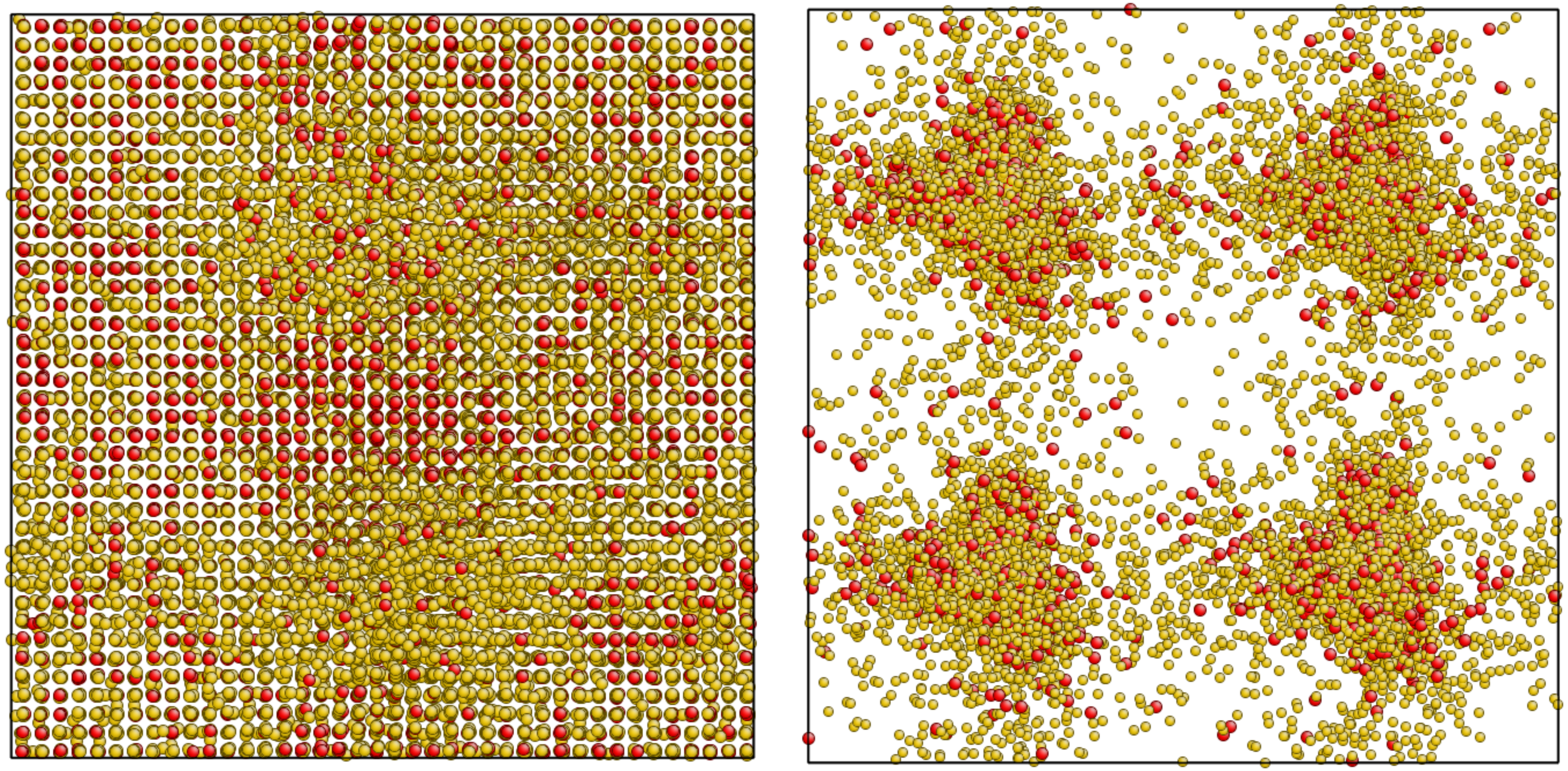
Input random configuration



Resultant artificial order

L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, *Acta Materialia,* 125 (2017) 15-26

Not accounting for instrumental decay function



L.R. Owen, H.Y. Playford, H.J. Stone, M.G. Tucker, *Acta Materialia,* 125 (2017) 15-26

Metallurgical challenges…

Mosaic

Effects of texture

Effect of crystallographic texture on pair distribution function analysis in engineering materials

Monika Rolinska[1]*, Lewis R. Owen[2], Yuanpeng Zhang[3], Peter Hedström[1], Matthew G. Tucker[3]

[1] Dept. of Materials Science and Engineering, KTH Royal Institute of Technology, Brinellvägen 23, 100 44, Stockholm, Sweden

[2] University of Sheffield, School of Chemical, Materials and Biological Engineering, Sir Robert Hadfield Building, Mappin Street, Sheffield S1 3JD, United Kingdom

[3] Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

* Corresponding author, email: rolinska@kth.se

Monika Rolinska

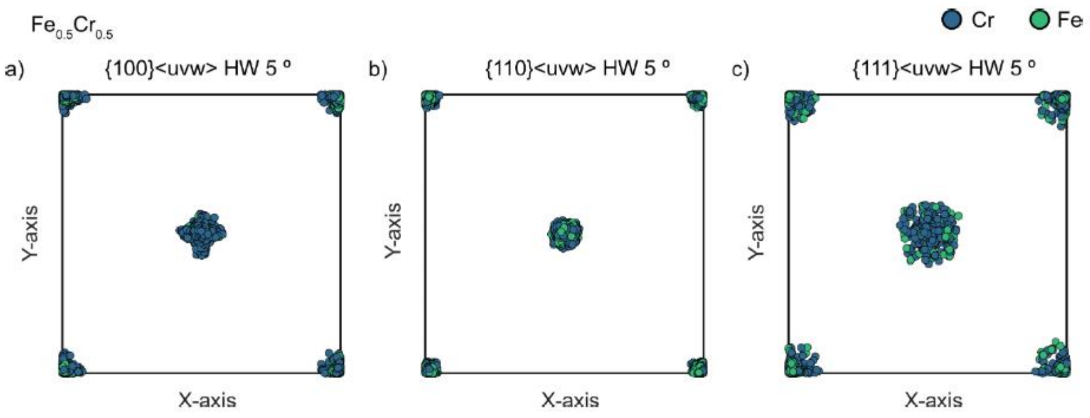


Figure 12 *Distortions on the collapsed supercells of $Fe_{0.5}Cr_{0.5}$ caused by different textures a) sharp {100}<uvw> texture b) sharp {110}<uvw> texture c) sharp {111}<uvw>texture*

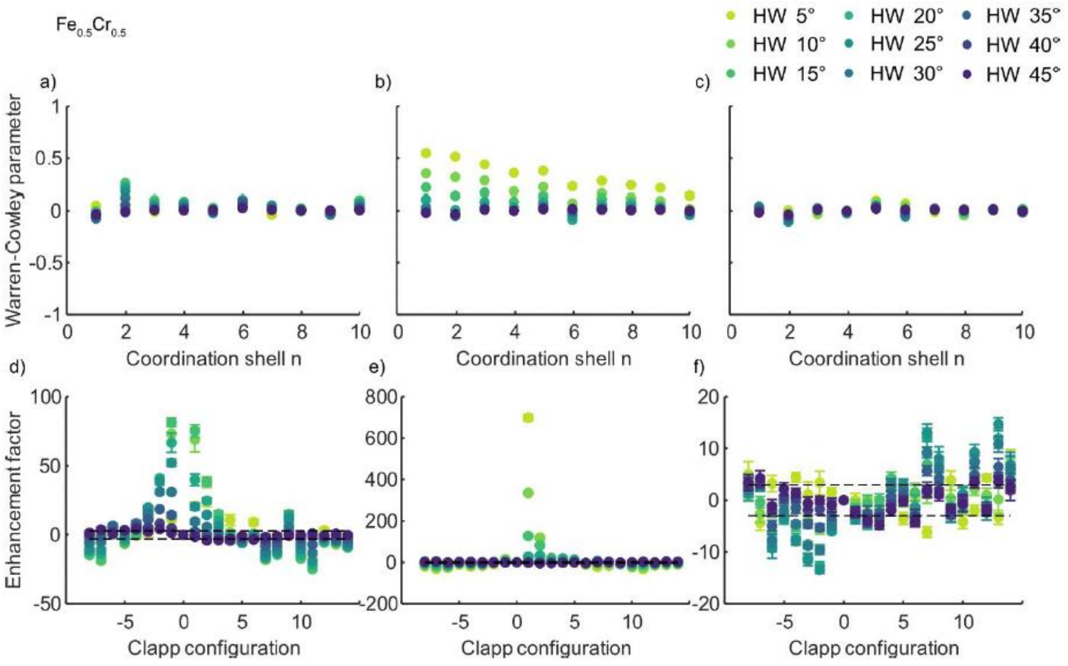


Figure 10 *Average of 10 runs showing the Warren-Cowley parameters for the first 10 coordination shells (a-c) and Clapp configurations enhancement factors (d-f) for different applied textures in the $Fe_{0.5}Cr_{0.5}$ system*

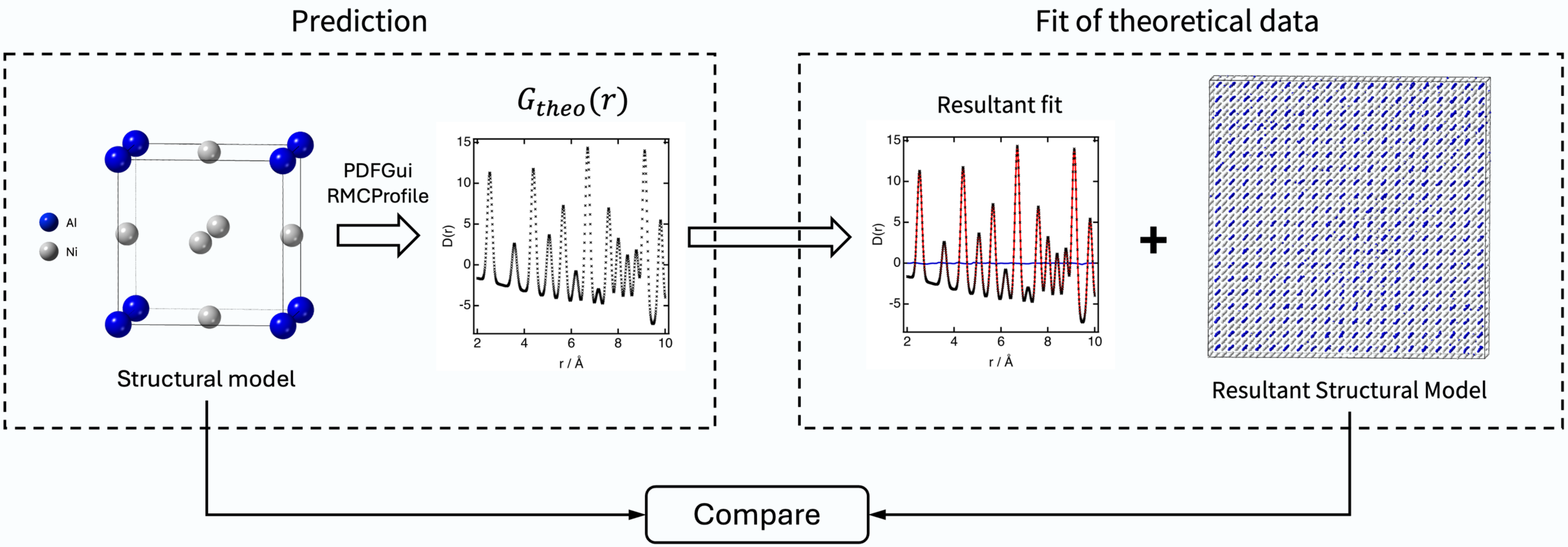
Methods

Running RMC

Mosaic

- Run with multiple starting configurations
- Run multiple times (and compare similarities)
- Testing and simulation

Simulate – test the concept

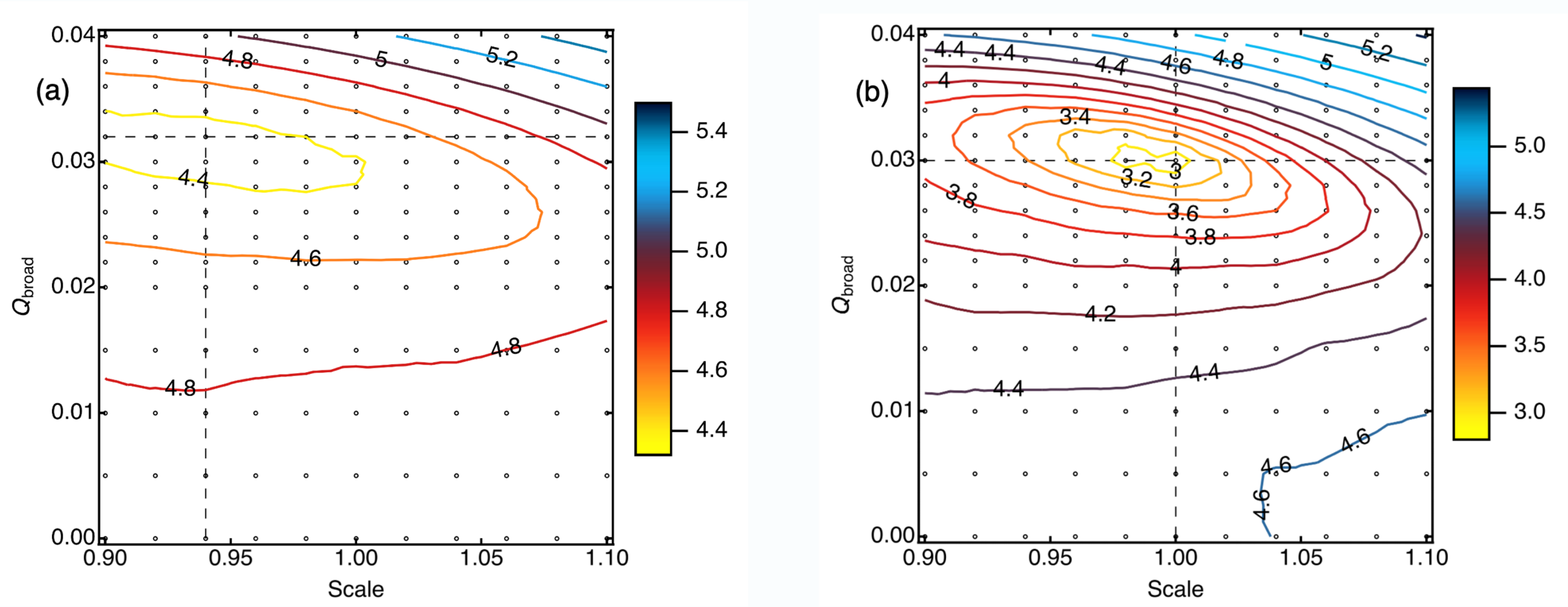


Running RMC

- Run with multiple starting configurations
- Run multiple times (and compare similarities)
- Testing and simulation
- Vary the parameter space
  - (particularly the important parameters)
  - Look for signs of issues

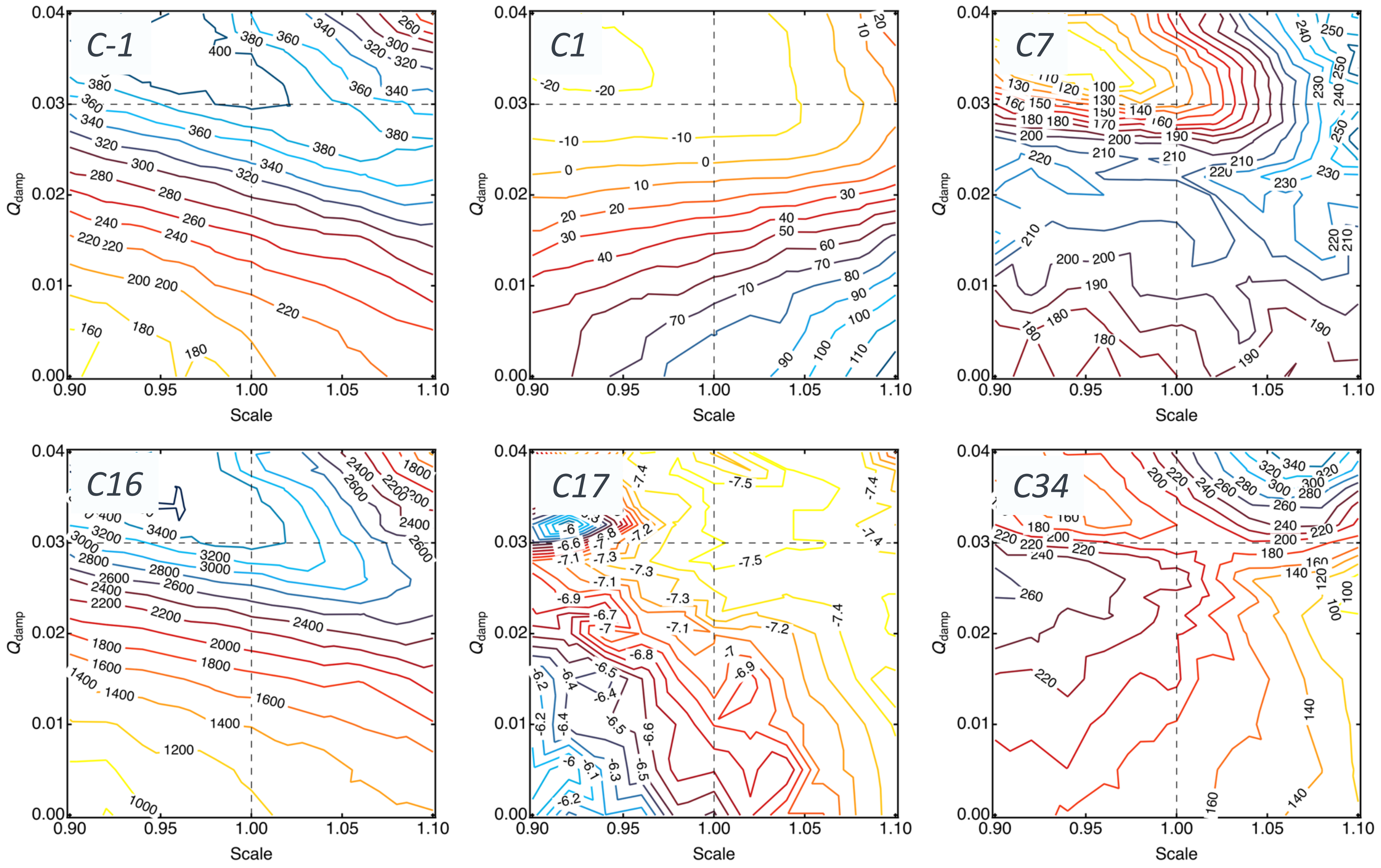
Varying the parameters

Mosaic



Stability to changes in parameters

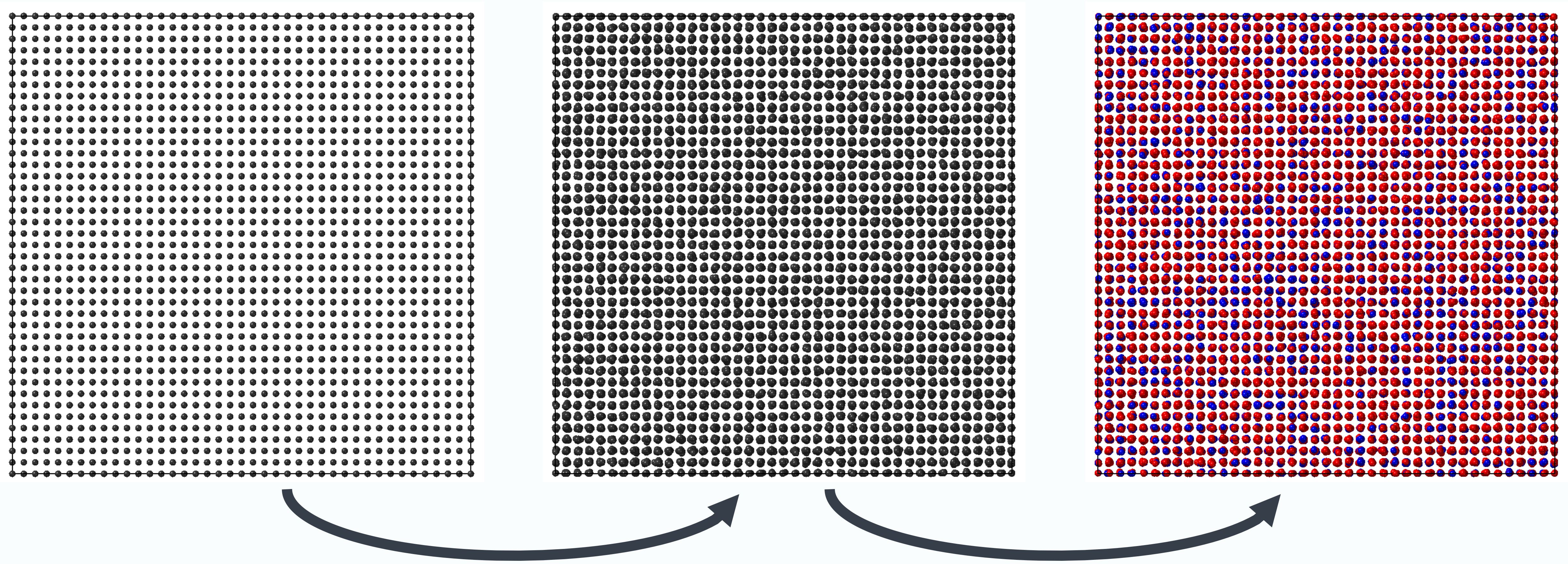
Mosaic



Running RMC

- Run with multiple starting configurations
- Run multiple times (and compare similarities)
- Testing and simulation
- Vary the parameter space
    - (particularly the important parameters)
    - Look for signs of issues
- Try ‘Grey atom’ method

Grey atom refinement



Translations only

Colour then allow swaps

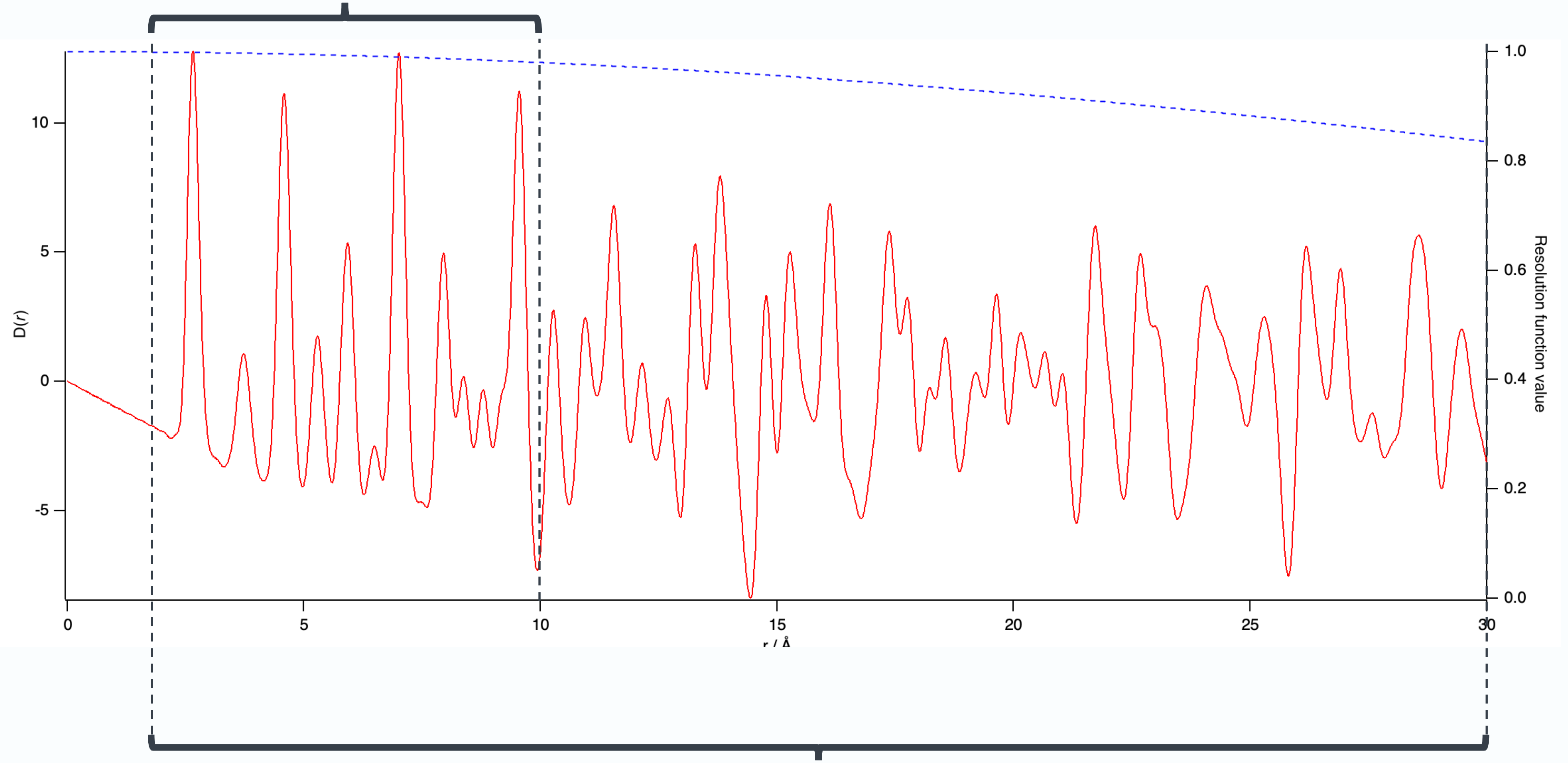
Running RMC

Mosaic

- Run with multiple starting configurations
- Run multiple times (and compare similarities)
- Testing and simulation
- Vary the parameter space
  - (particularly the important parameters)
  - Look for signs of issues
- Try ‘Grey atom’ method
- Vary the fitting regime
  - Datasets
  - Weightings
  - Regions

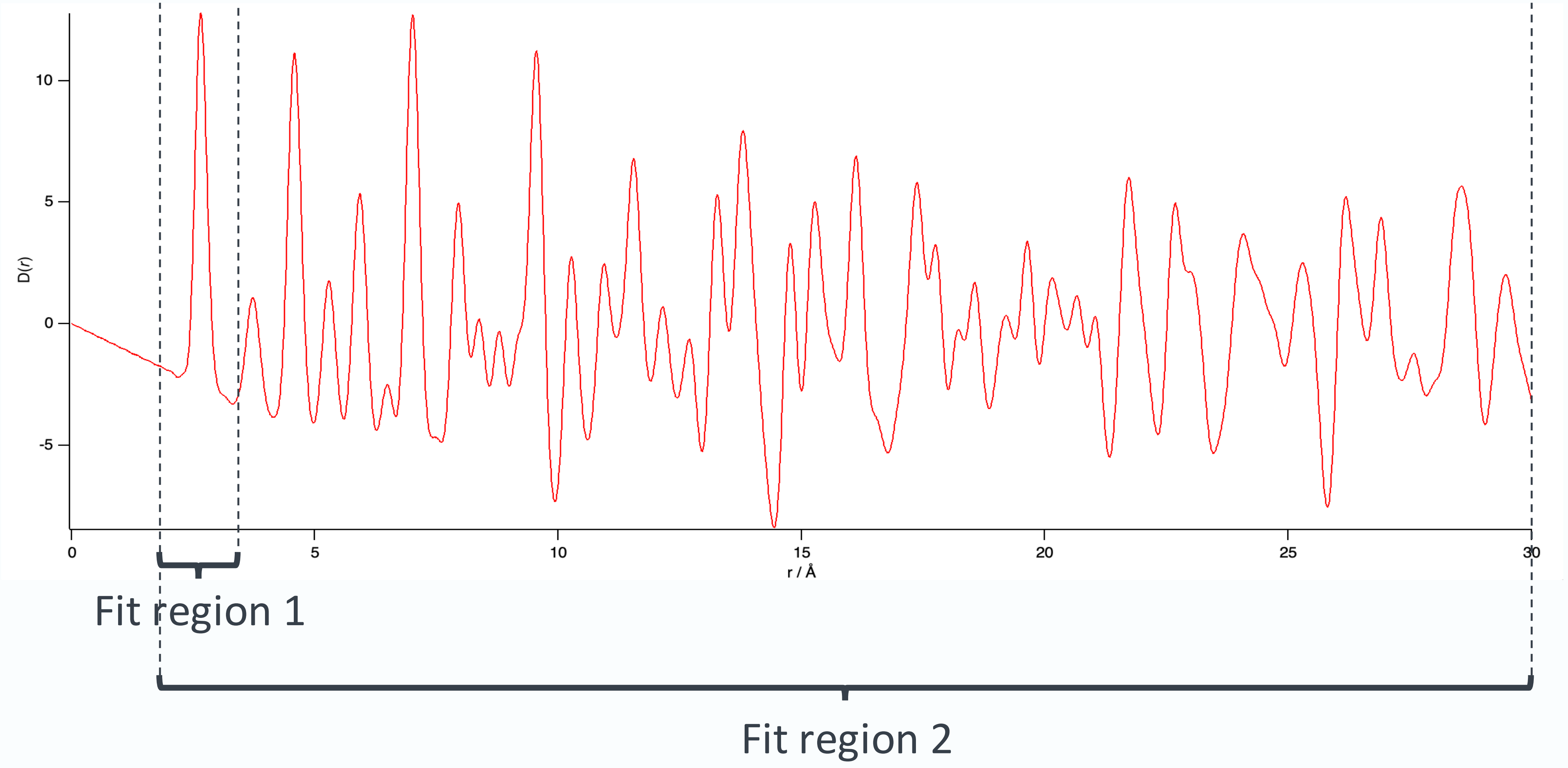
Fitting regions – preliminary fitting

Test region 1



Test region 2

Fitting regions – Multiple region fit



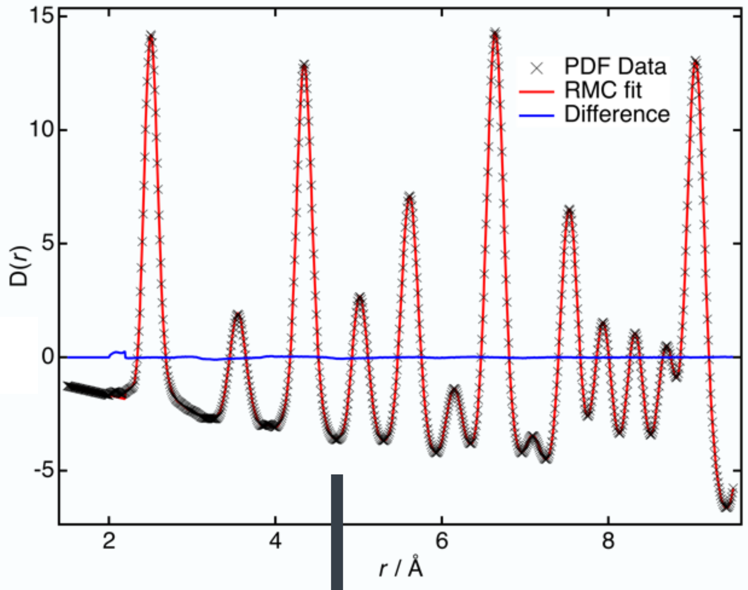
Running RMC

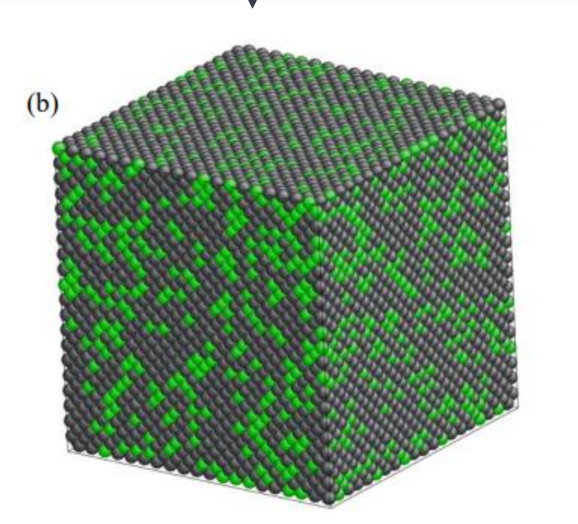
Mosaic

- Run with multiple starting configurations
- Run multiple times (and compare similarities)
- Vary the parameter space
    - (particularly the important parameters)
    - Look for signs of issues
- Try ‘Grey atom’ method
- Vary the fitting regime
    - Datasets
    - Weightings
    - Regions

Opportunities

Ni_2Cr – K-state





614 H. G. Baer: Überstruktur und K-Zustand im System Nickel-Chrom Z. Metallkde.

Überstruktur und K-Zustand im System Nickel-Chrom*)**)

Von Hans Günter Baer in Hanau a.M.

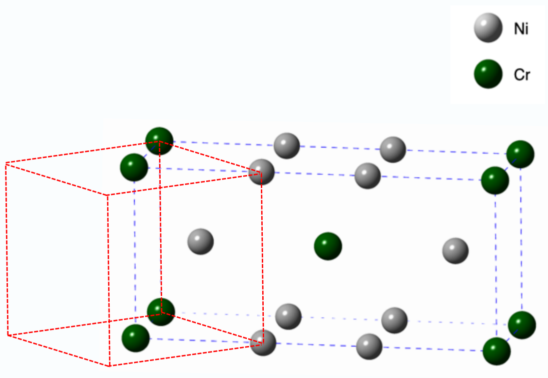
(Aus dem Laboratorium der Vacuumschmelze AG., Hanau)

Versuchsdurchführung — Röntgenographischer Nachweis der Ordnungsphase Ni_2Cr — Existenzgebiet von Ni_2Cr und Bildungskinetik — Neubestimmung der Löslichkeitslinie für Chrom in Nickel — Folgerungen

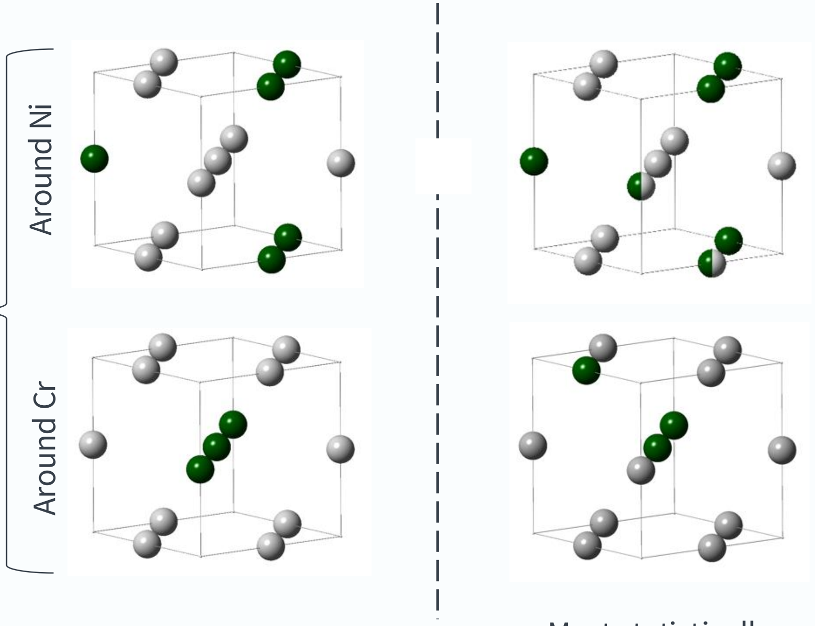
Die homogenen Mischkristalle mancher Metalle, z. B. Nickel mit Chrom, Molybdän oder Aluminium, Eisen mit Aluminium, Kupfer mit Nickel, oder ternäre Legierungen, wie Nickel-Chrom-Eisen, Eisen-Aluminium-Chrom oder Kupfer-Nickel-Zink, zeigen Anomalien in ihren physikalischen Eigenschaften, für deren Charakterisierung sich nach dem Vorschlag von H. Thomas[1]) der Begriff K-Zustand eingebürgert hat. Nach der von ihm stammenden ausführlichen

gung bei einer Legierung, die 20 At.-% Cr enthielt und die nach einer Vorglühung längere Zeit in der Gegend von 500° getempert worden war, eine Nahordnung nachzuweisen. Sie kommen zu dem Schluß, daß ein hoher Grad von Nahordnung nicht vorhanden sein kann.

Die Verknüpfung des K-Zustandes mit einer Änderung des Auffüllungsgrades der inneren Elektronenschalen im Sinne eines Elektronenrücktritts allein



Ni_2Cr



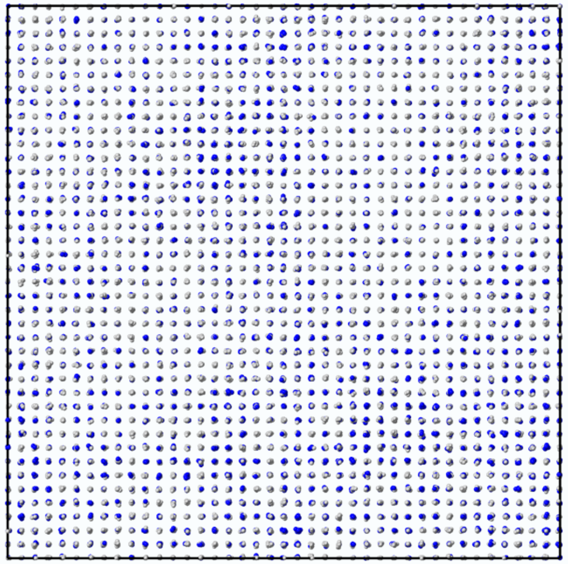
Expected for Ni_2Cr structure

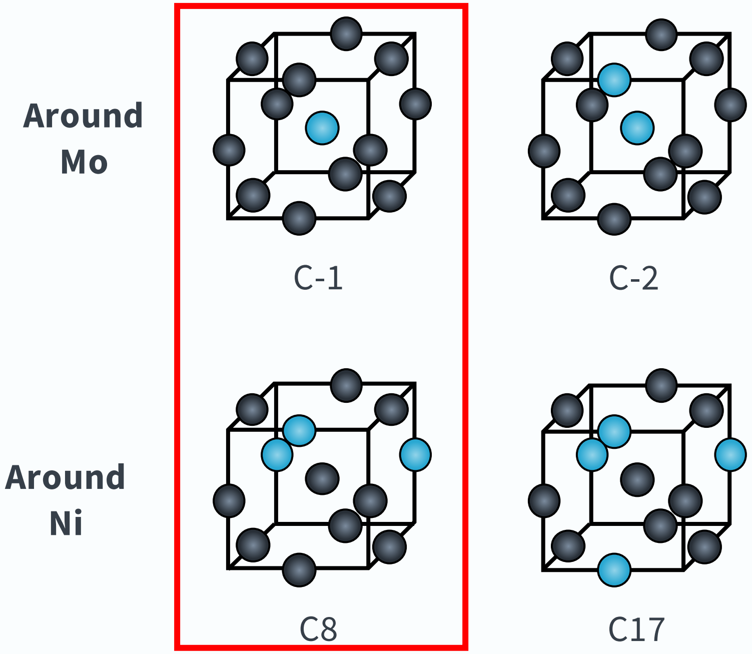
Most statistically increased local configurations

B.S. Rowlands, L.R. Owen, J.R. Miller, X. Shen, W.Song, H.J. Stone, E.I. Galindo-Nava, T. Jackson & C.M.F. Rae. The PLC Effect in the Absence of Long-Range Cottrell Atmospheres in RR1000. In: Cormier, J., et al. Superalloys 2024. ISS 2024. The Minerals, Metals & Materials Series. Springer, Cham. https://doi.org/10.1007/978-3-031-63937-1_37

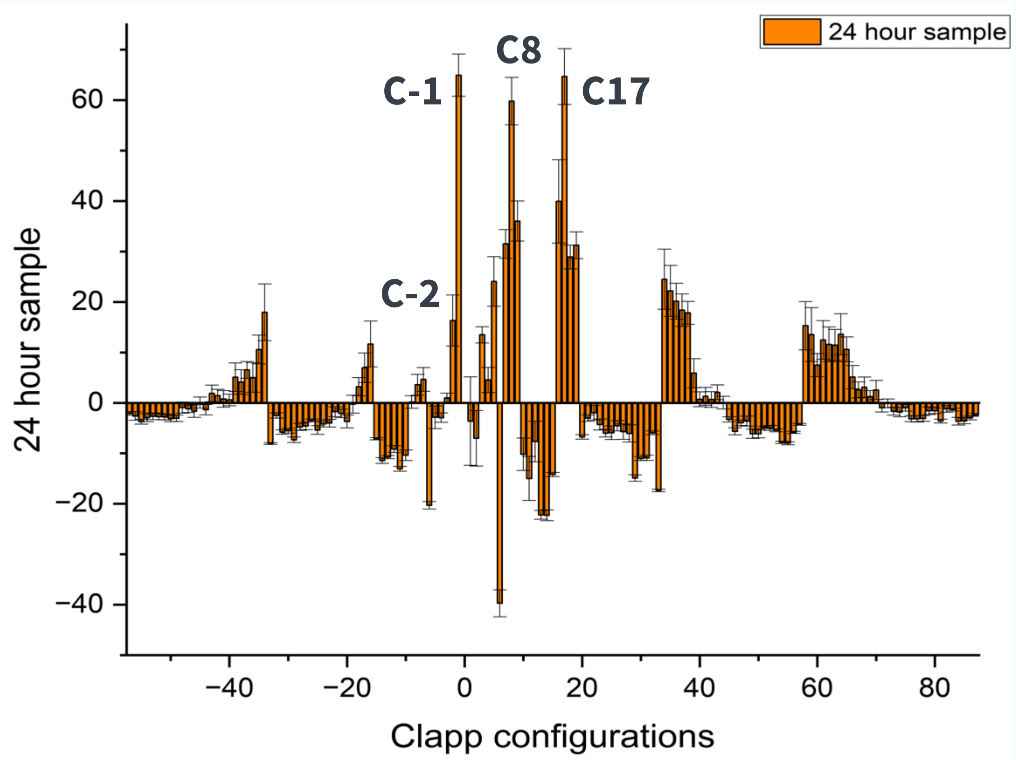
Ni_4Mo – Following the phase transition

Niels Schreiner





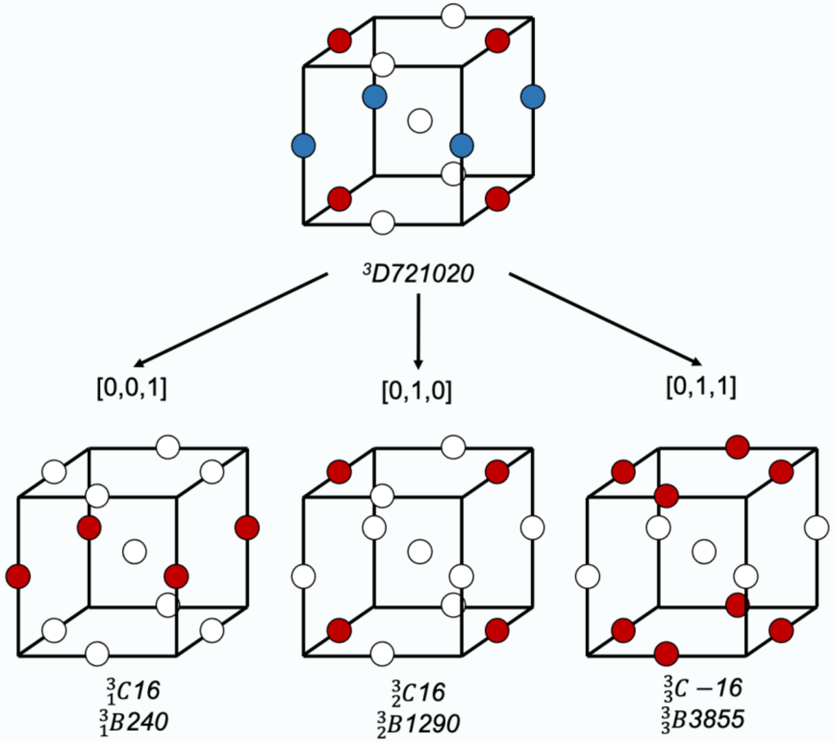
D1a key configurations

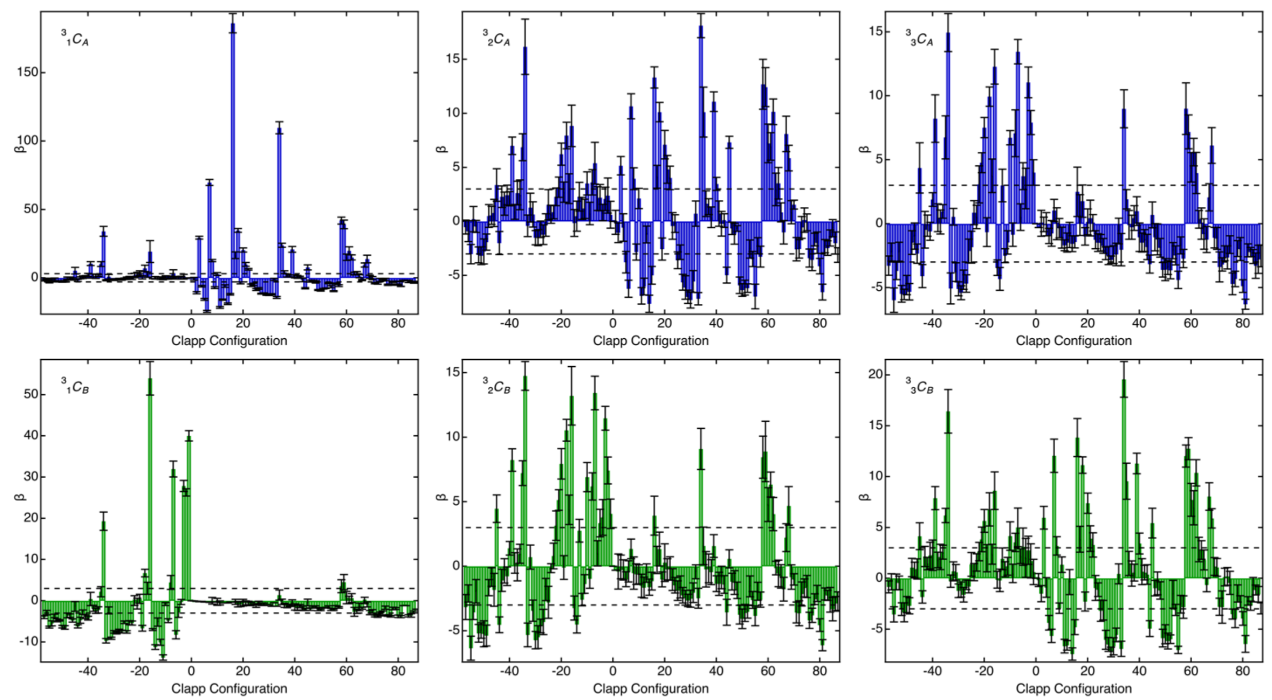


"Understanding the ordering transition and local structure states in Ni_4Mo using neutron total scattering" – N. Schreiner, P.C. Chater, L.R. Owen, Manuscript in preparation.

Multicomponent systems

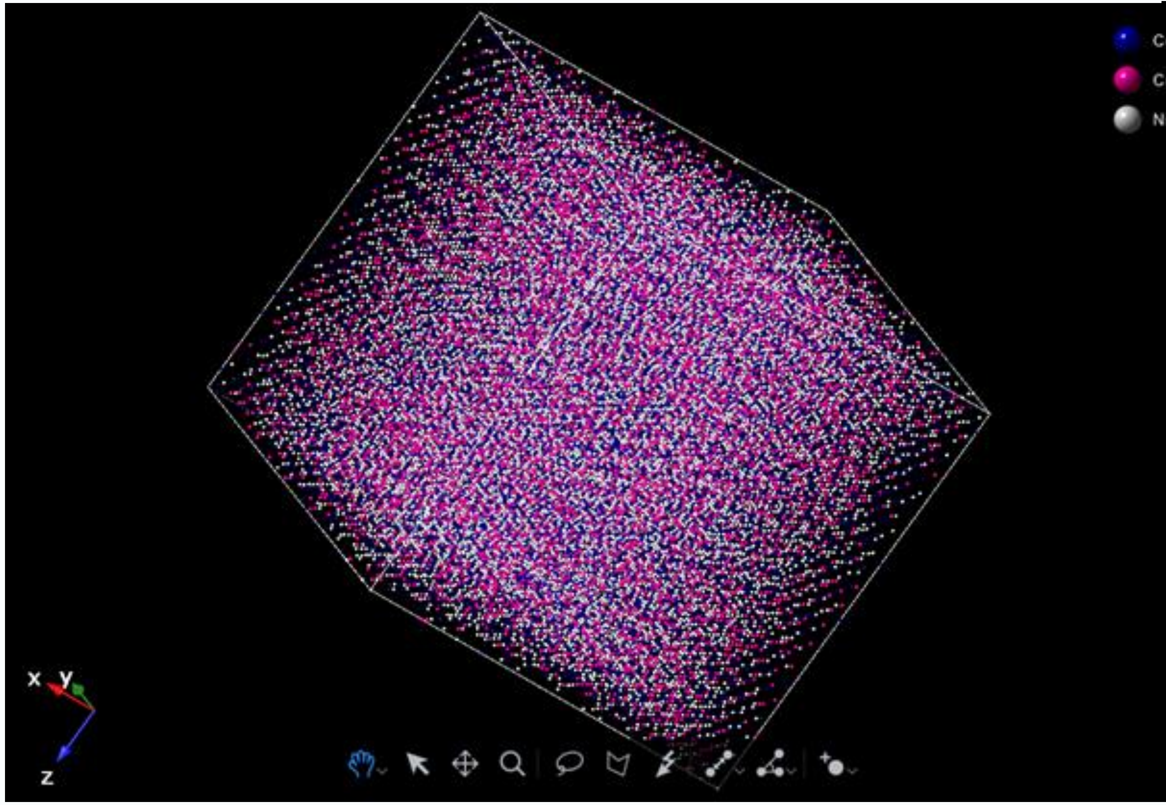
Mosaic

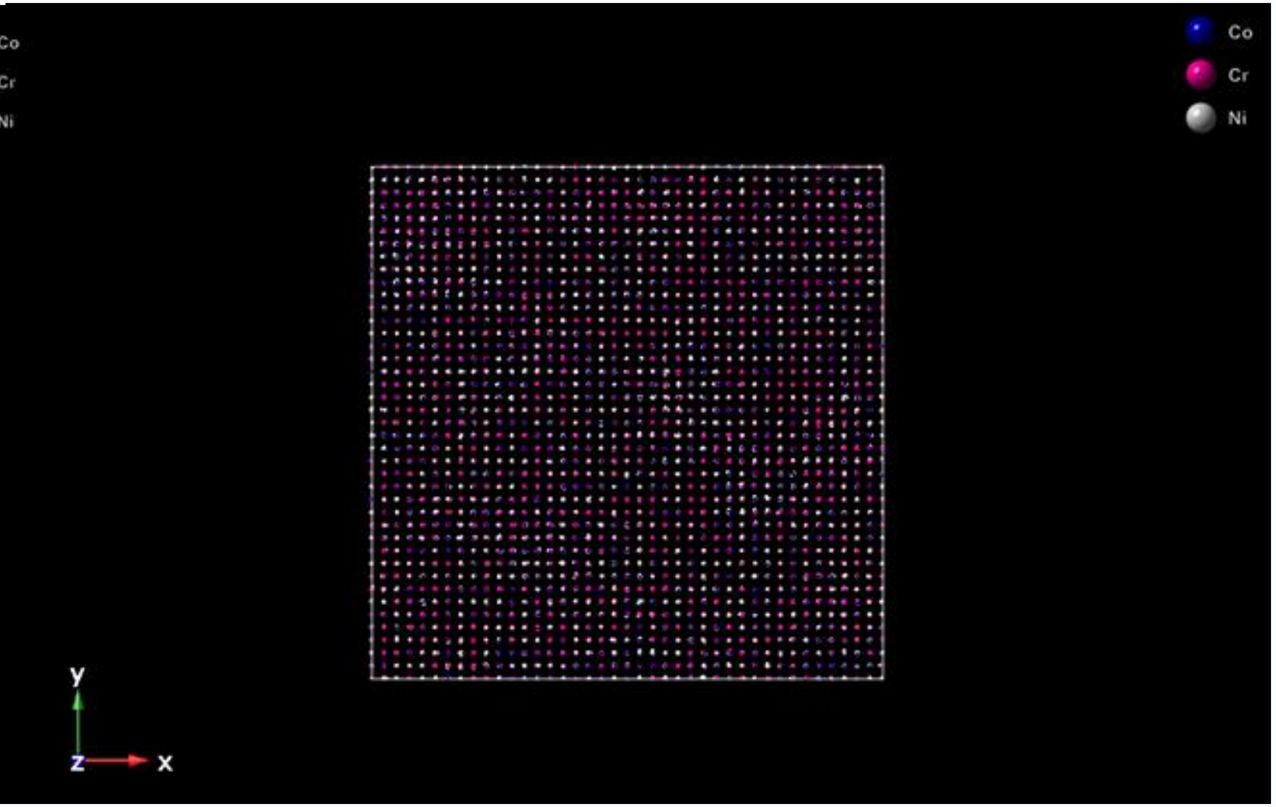




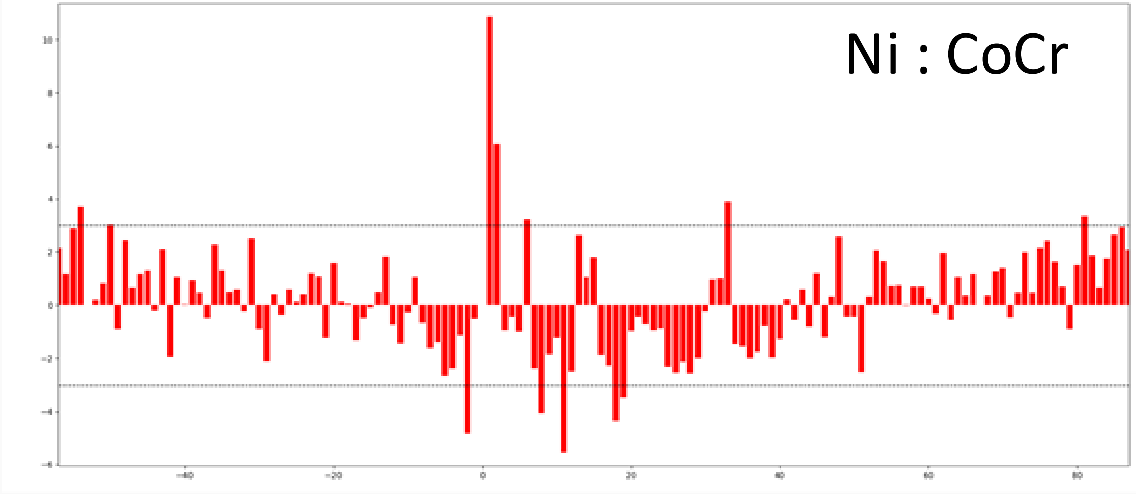
To higher order systems - NiCoCr

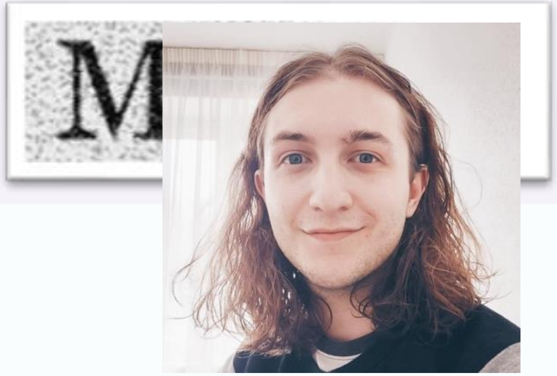
Ben Jolly



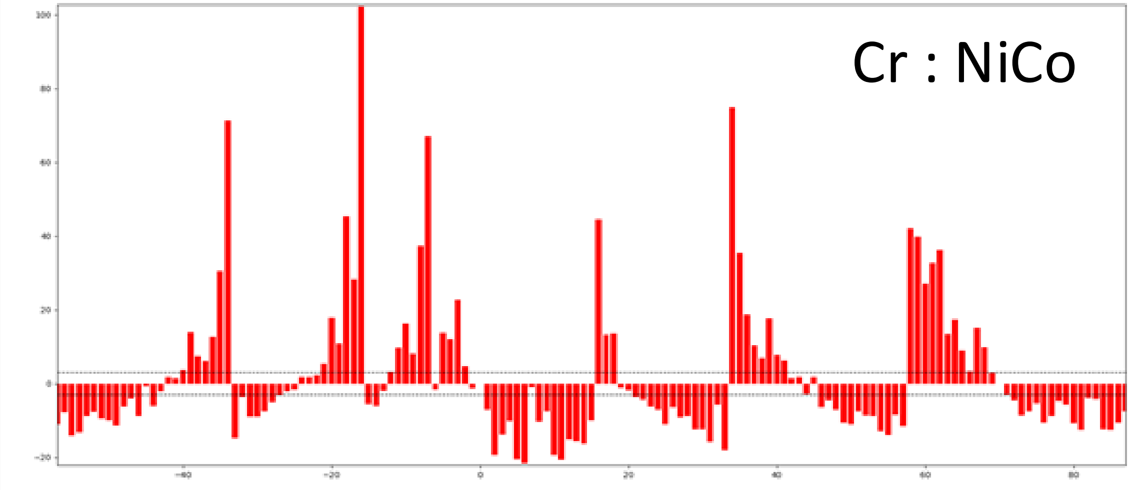


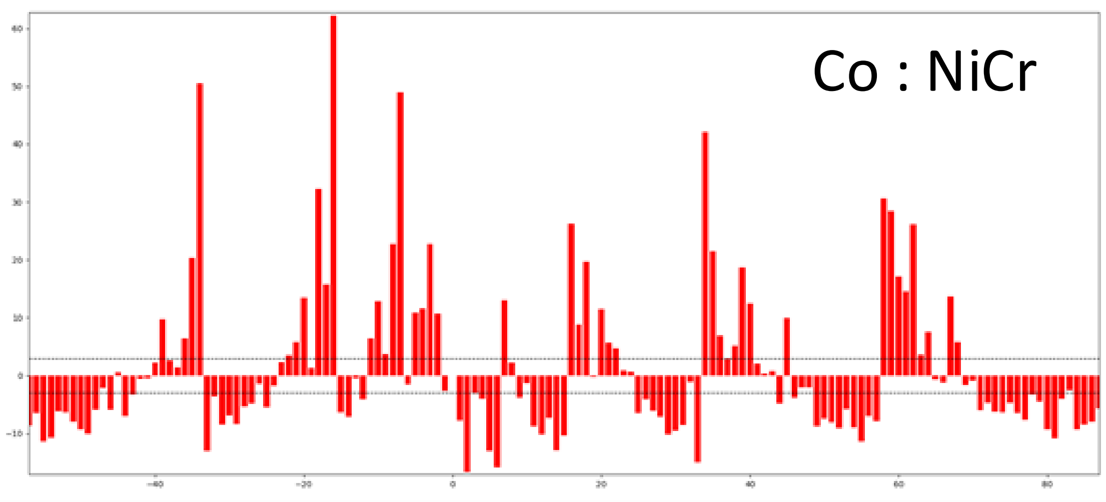
To higher order systems - NiCoCr





Ben Jolly



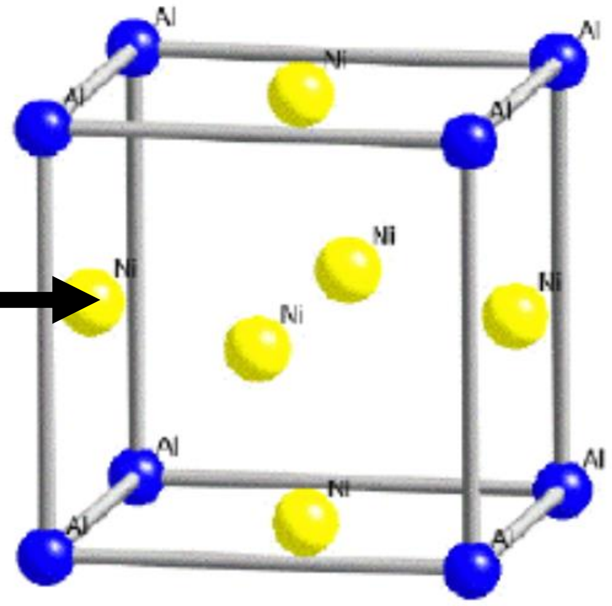


Sublattice ordering in $L1_2$ alloys

Mosaic

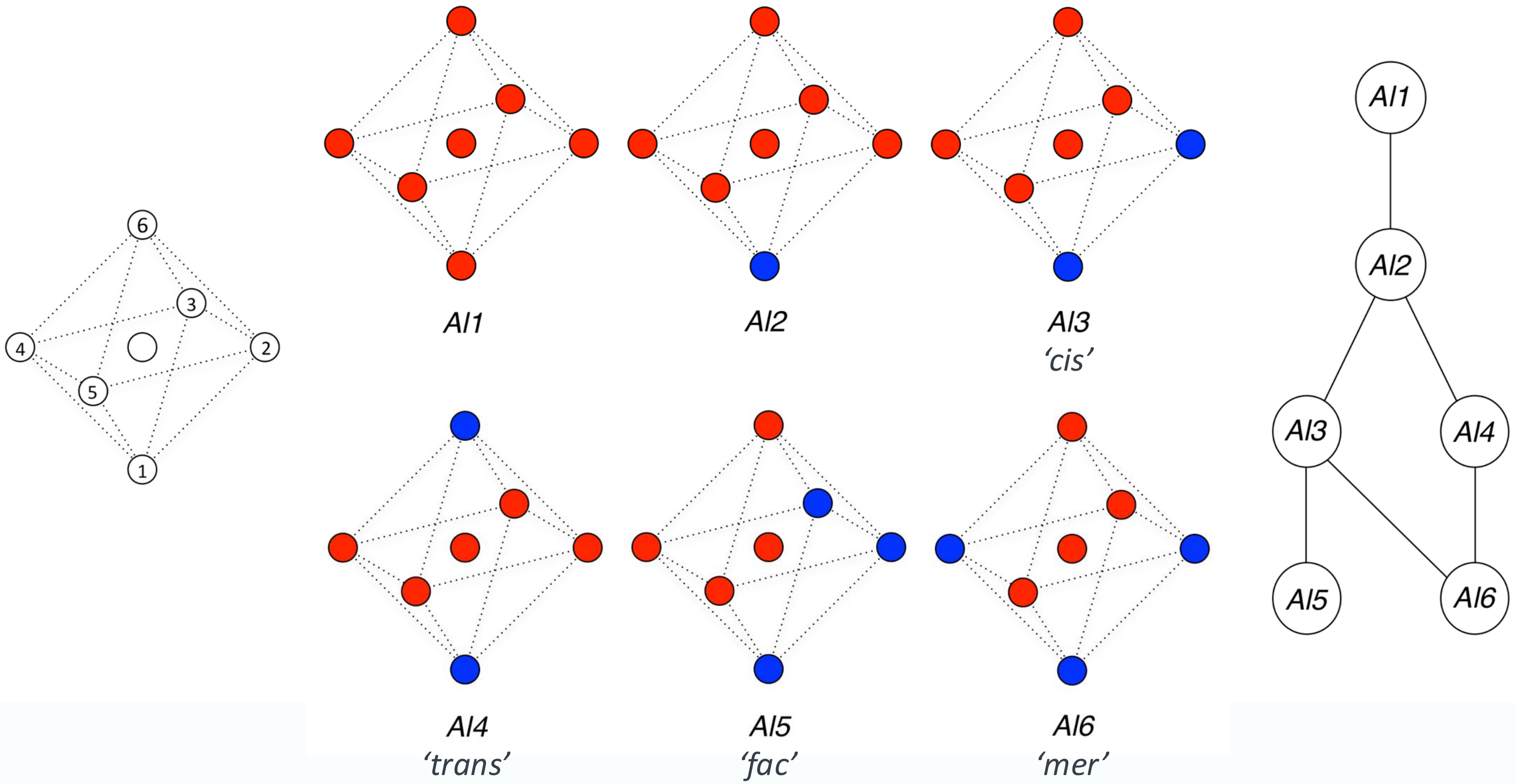
Ti, Ta, Nb

Co

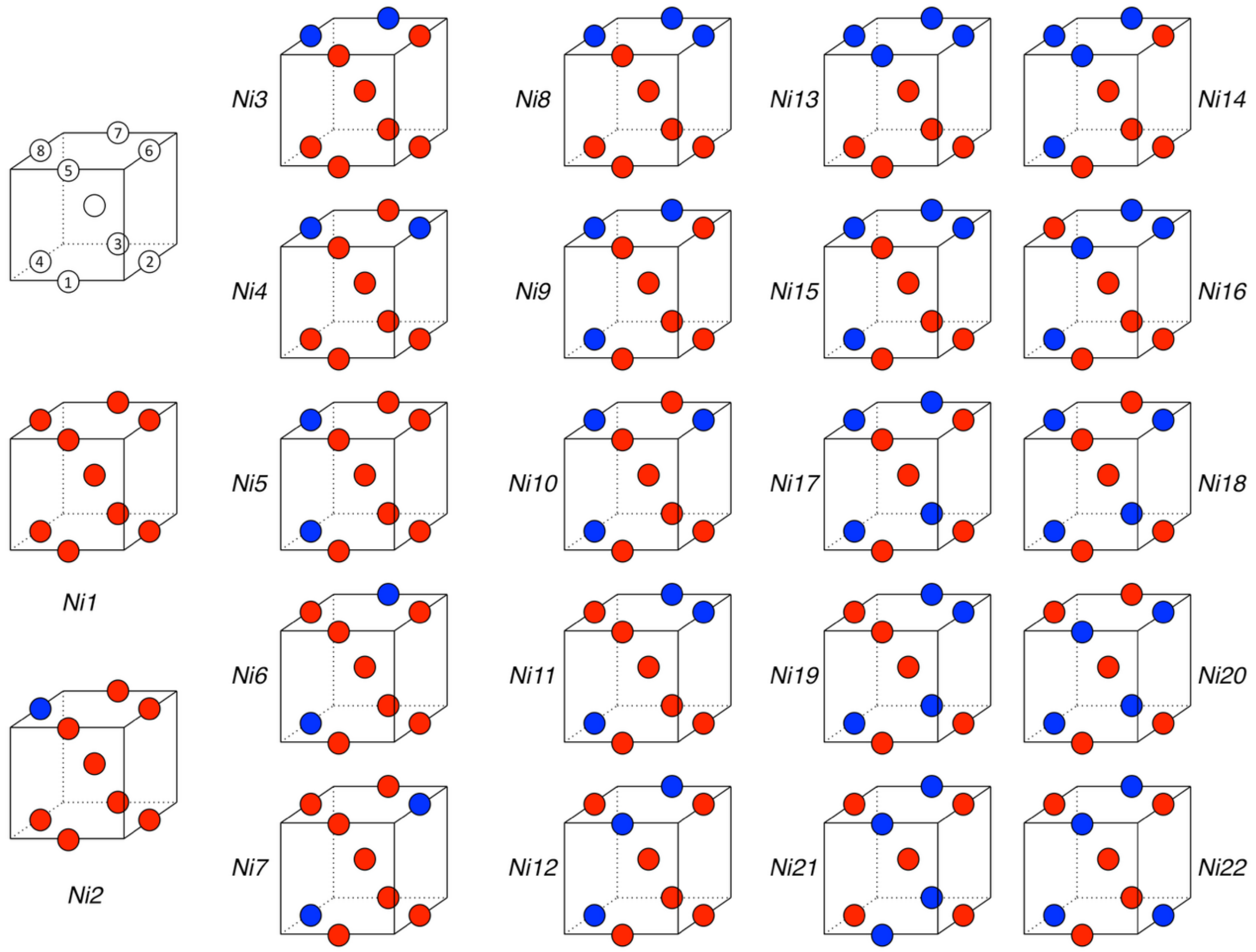


Crystal structure of γ'

Aluminium sublattice

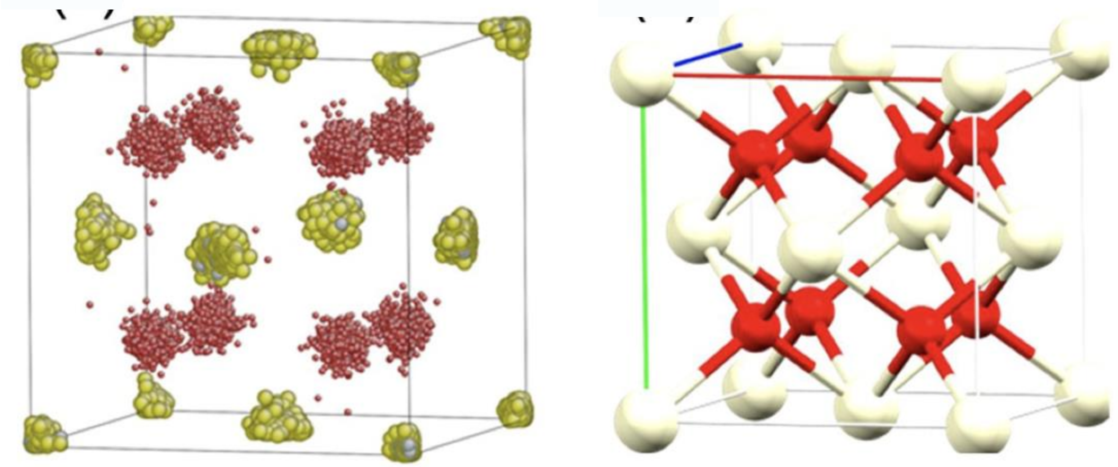


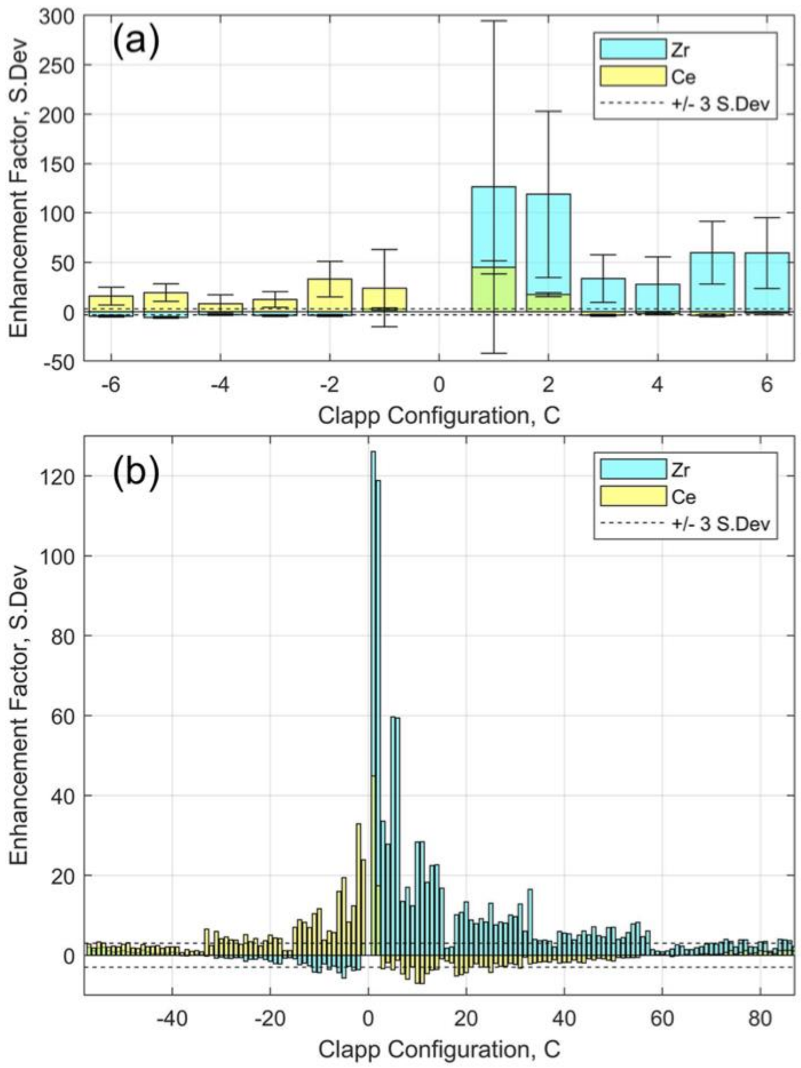
Nickel sublattice



Chemical systems

Mosaic





RESEARCH ARTICLE | MARCH 21 2023

Order and disorder in cerium-rich ceria-zirconia solid solutions revealed from reverse Monte Carlo analysis of neutron and x-ray total scattering

Special Collection: Challenges and Perspectives in Materials Chemistry—A Celebration of Prof. Sir Anthony K. Cheetham's 75th Birthday

Aron Summer; Helen Y. Playford; Lewis R. Owen; Janet M. Fisher; Amy Kolpin; David Thompsett; Richard I. Walton

Check for updates

APL Mater. 11, 031113 (2023)
https://doi.org/10.1063/5.0139567

Thank you for listening

Mosaic

Acknowledgements

Ben Jolly (University of Sheffield)

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Prof. Howard Stone (Department of Material Science and Metallurgy, University of Cambridge)

Dr. Matt Tucker (Oak Ridge National Laboratory)

Funding:

I would like to acknowledge ongoing support from the Royal Academy of Engineering during my Research Fellowship

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Royal Academy of Engineering

EPSRC Engineering and Physical Sciences Research Council

Science & Technology Facilities Council ISIS

Gonville & Caius UNIVERSITY OF CAMBRIDGE

Shameless plug

Mosaic

British Crystallographic Association Spring Meeting 2026

30th Mar– 1st April 2026

University of Leeds

Abstract deadline

Monday 19th Jan 2026

Plenaries:

BSG :	Dr Basil Greber
CCG:	Prof Neil Champness
ESCG:	Dr Ines Collings
IG:	Prof John Helliwell
PCG:	Prof Abbie Mclaughlin

Sessions include:

(BSG) Structure-Based Drug Discovery
(BSG) Complex structures
(IG/BSG) Complementary techniques/Disorder
(CCG/IG/ESCG) Crystal Formation (Crystallisation/Crystal prediction/Crystal Engineering)
(CCG) George Sheldrick: his life and impact
(CCG) Investigating molecular crystals
(PCG/CCG) Functional materials
(PCG) Quantum Materials
(PCG) Energy materials
Open sessions in all areas!!

Thank you for listening

Mosaic

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