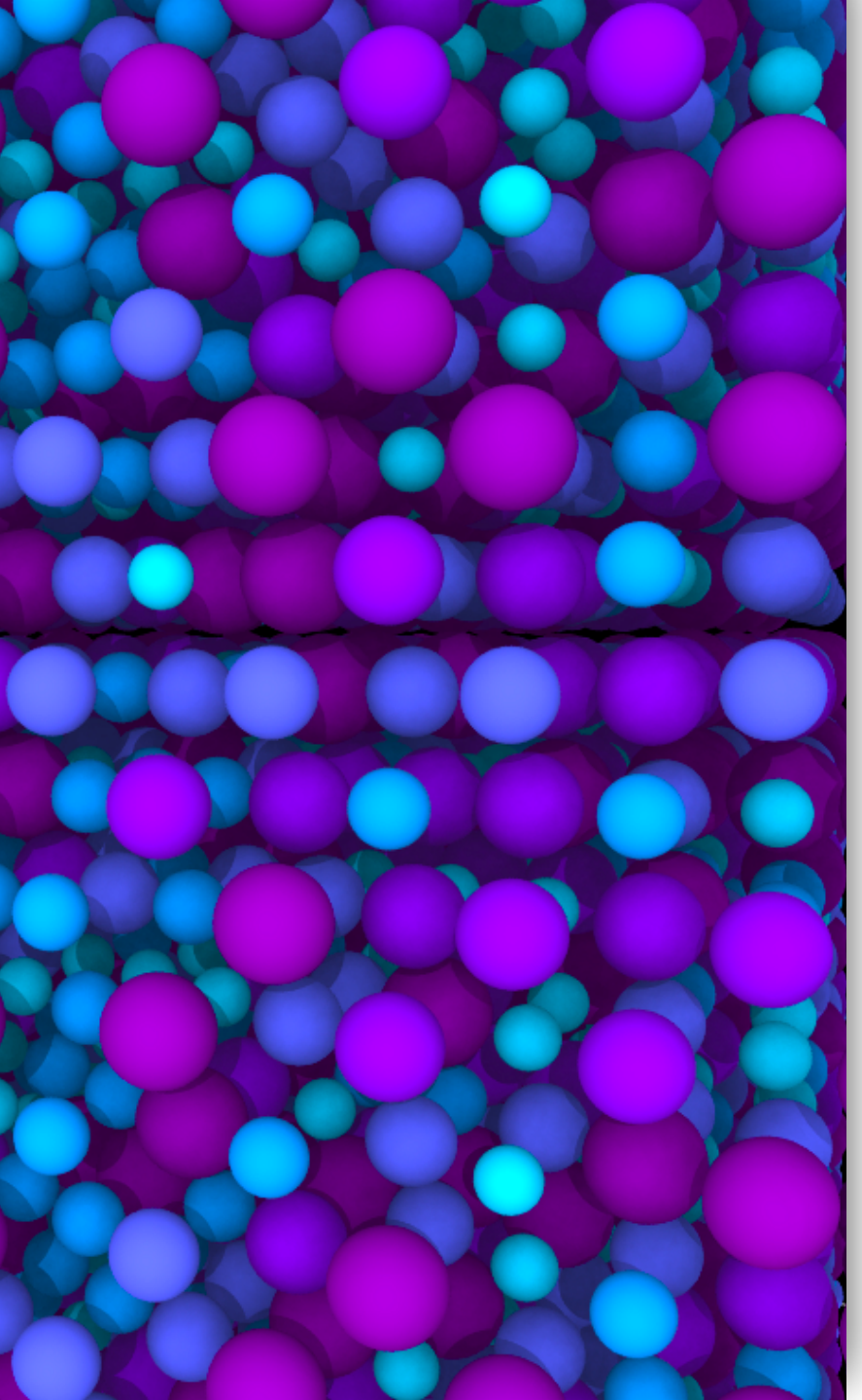

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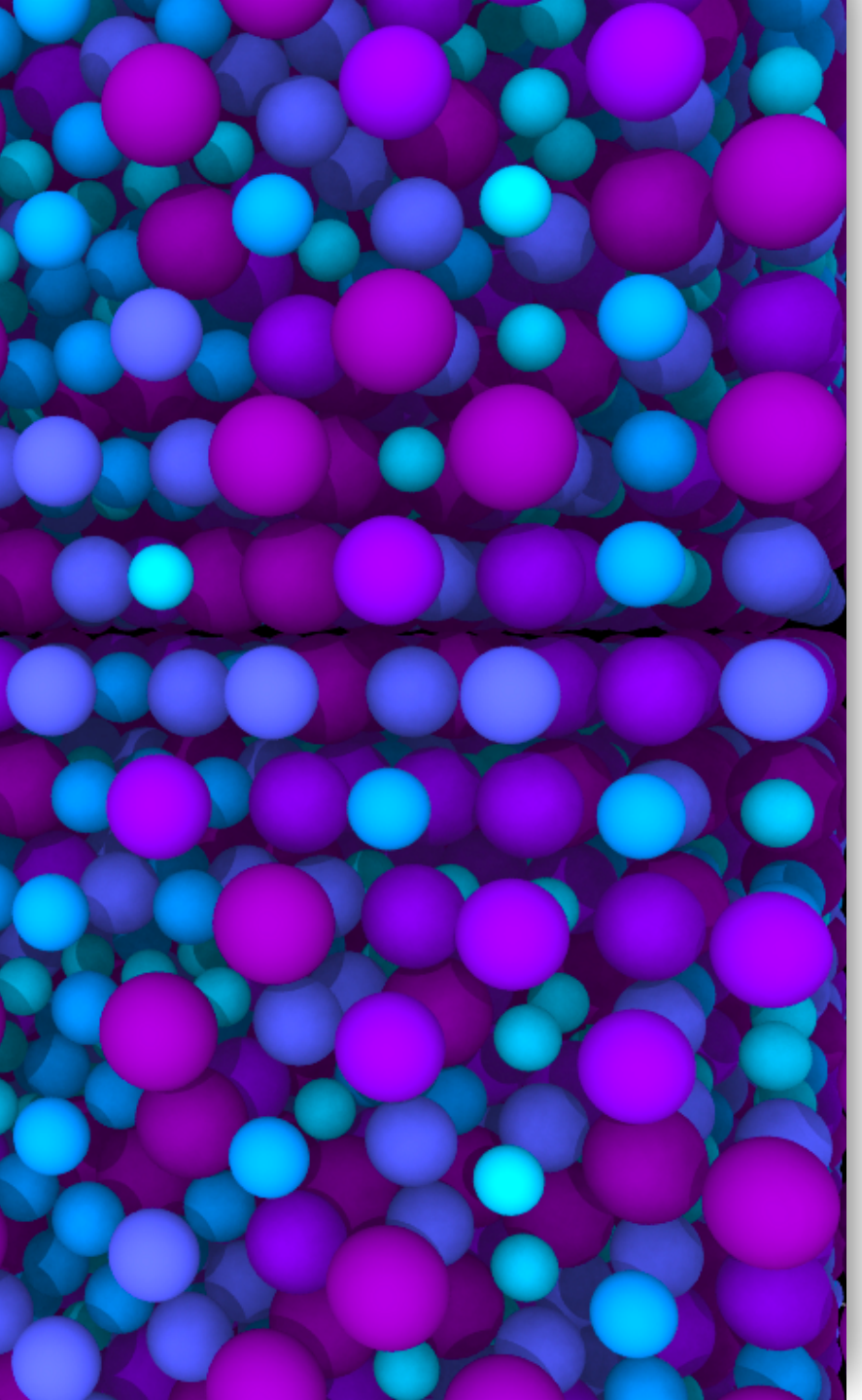
QUASI-LOCALIZED MODES IN CRYSTALLINE HIGH ENTROPY ALLOYS

Silvia Bonfanti

NOMATEN

Interaction, Disorder, Elasticity workshop – École de Physique des Houches – April 2-7, 2023



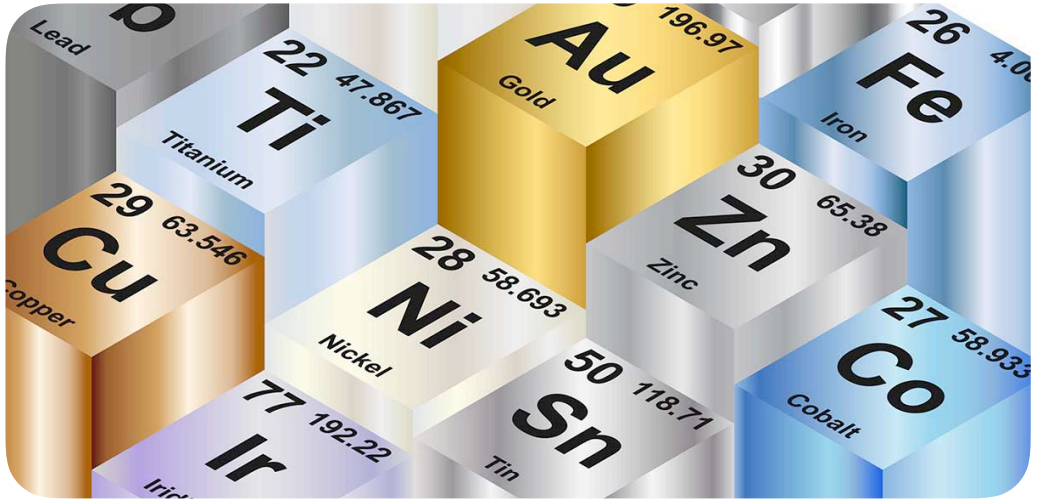
Outline

- High Entropy Alloys
- Microscopic Structure
- Vibrational Properties
- Disorder
- Future perspectives

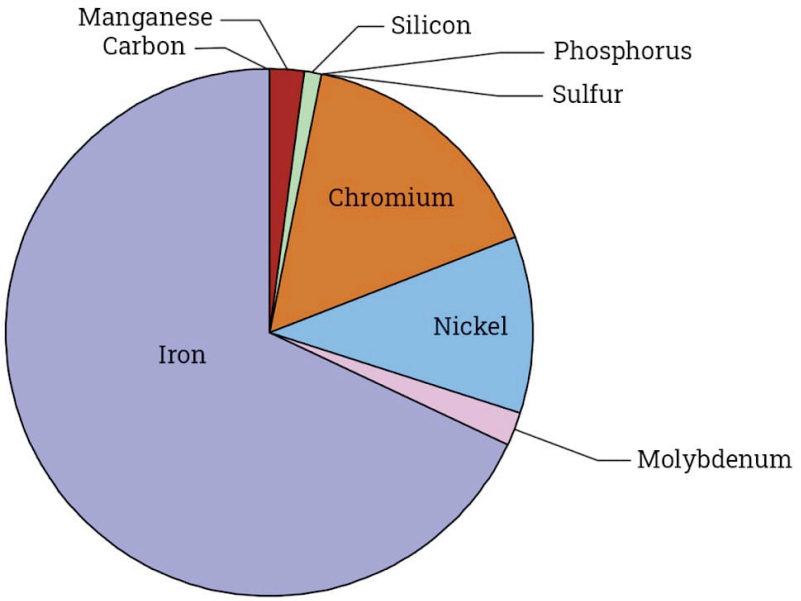
TRADITIONAL ALLOYS

ONE/TWO MAJOR METALLIC ELEMENTS
+ SMALLER AMOUNT OF MINOR ELEMENTS

Different alloy families



E.g.: Stainless Steel Composition

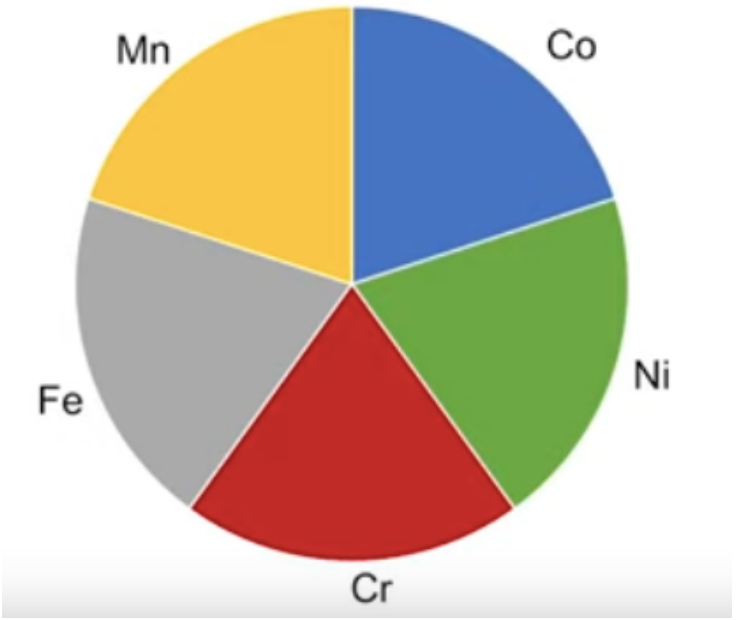


HIGH ENTROPY ALLOYS (2004)

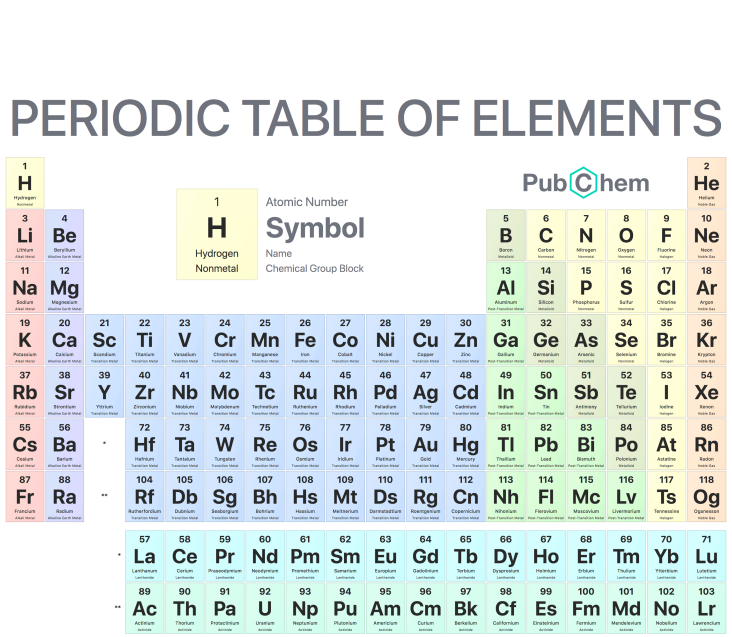
PROF. YEH @ UNI TAIWAN

PROF. CANTOR @ CALTECH

THE IDEA:
MIX SEVERAL (>4) SPECIES
IN SAME PROPORTION!

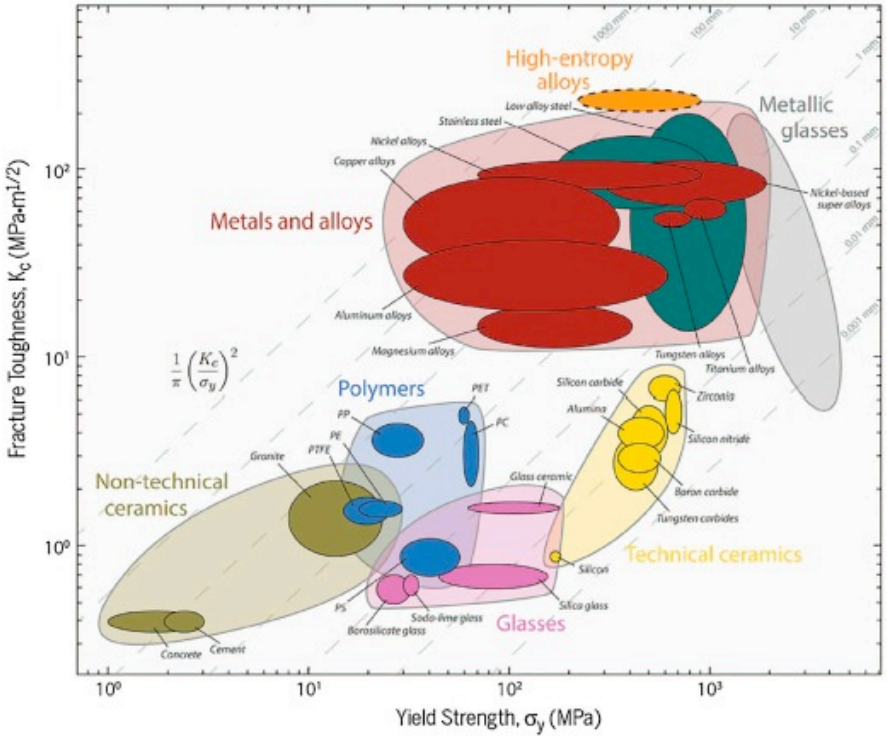


HIGH ENTROPY ALLOYS = IMPROVED PROPERTIES



50 METALS:
INFINITE POSSIBILITIES
OF COMBINATION

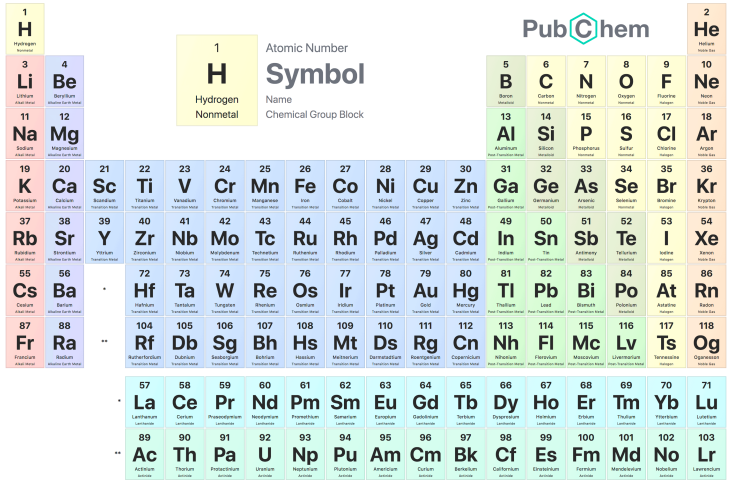
HIGH ENTROPY OF MIXING
ALTER THE INTERACTION
OF ELEMENTS:
COCKTAIL EFFECT



MECHANICAL
THERMODYNAMIC
CORROSION RESISTANCE...

HIGH ENTROPY ALLOYS = IMPROVED PROPERTIES

PERIODIC TABLE OF ELEMENTS



50 METALS:
INFINITE POSSIBILITIES
OF COMBINATION

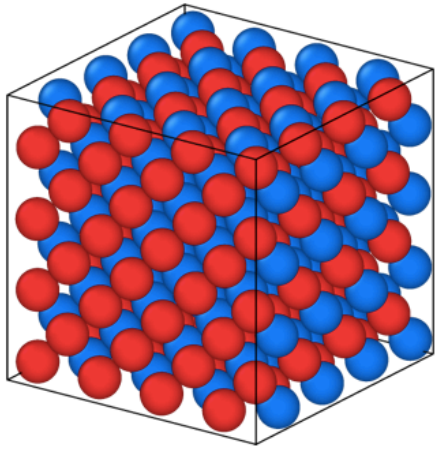
HIGH ENTROPY OF MIXING
ALTER THE INTERACTION
OF ELEMENTS:
COCKTAIL EFFECT

US: STRUCTURE-
PROPERTIES
HOW? MODELING (MD)

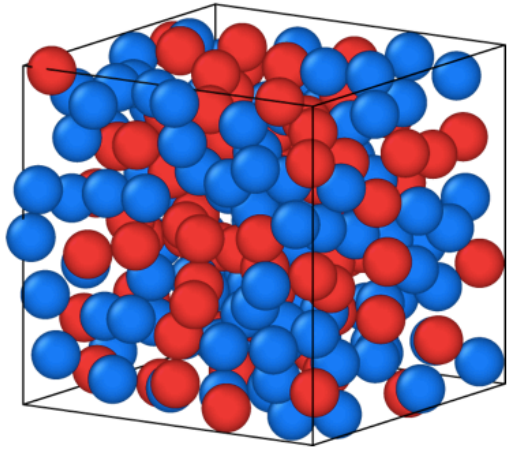
MICROSCOPIC STRUCTURE

CONVENTIONAL ALLOYS

CRYSTAL



GLASS

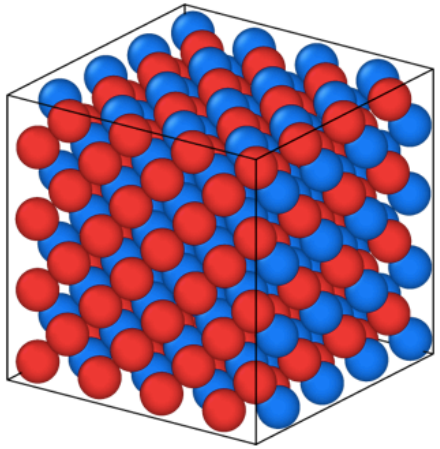


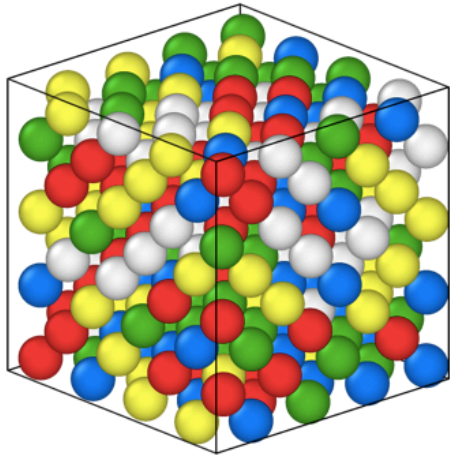
MICROSCOPIC STRUCTURE

CONVENTIONAL ALLOYS

HIGH ENTROPY ALLOYS

CRYSTAL

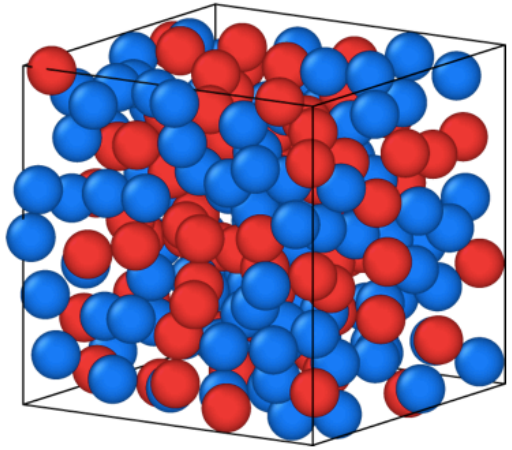




- POSITIONAL ORDER
- **COMPOSITIONAL DISORDER**

PARADIGM SHIFT

GLASS

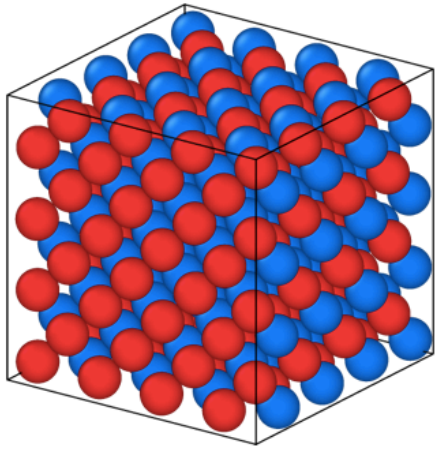


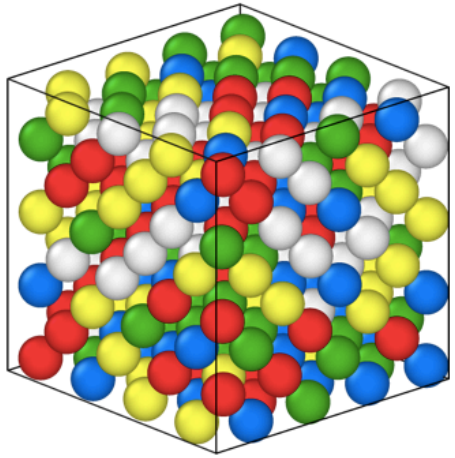
MICROSCOPIC STRUCTURE

CONVENTIONAL ALLOYS

HIGH ENTROPY ALLOYS

CRYSTAL





- POSITIONAL ORDER
- **COMPOSITIONAL DISORDER**

PARADIGM SHIFT

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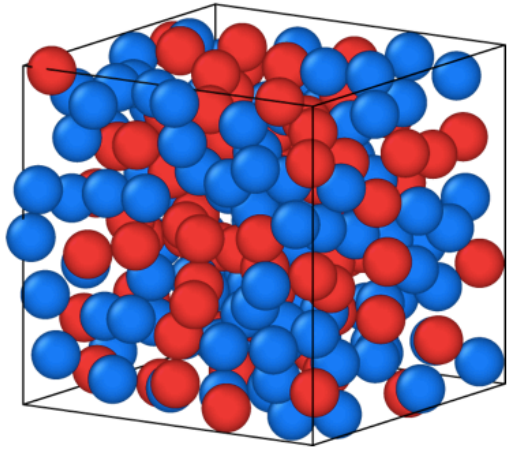
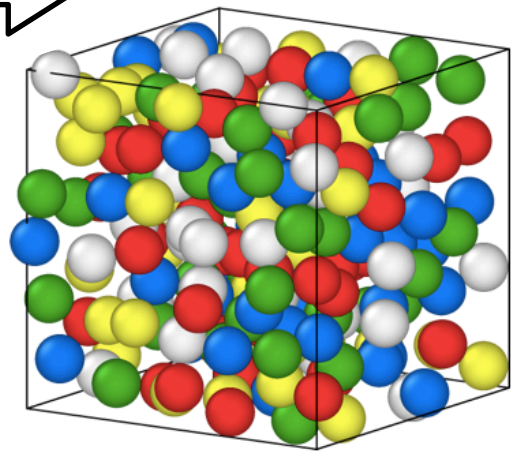




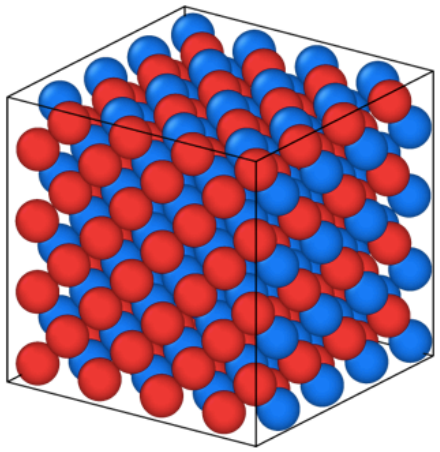
- POSITIONAL DISORDER

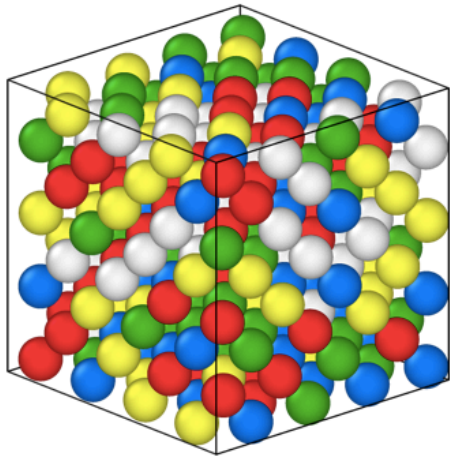
MICROSCOPIC STRUCTURE

CONVENTIONAL ALLOYS

HIGH ENTROPY ALLOYS

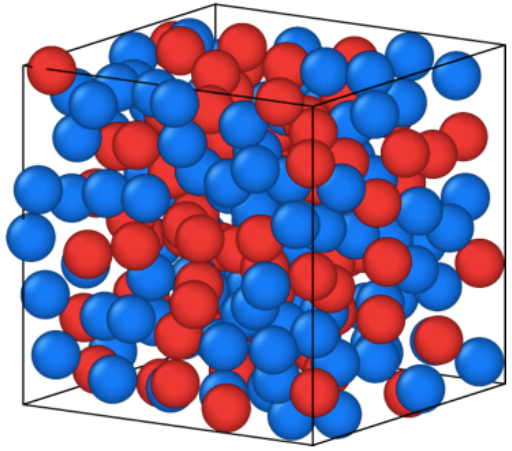
CRYSTAL

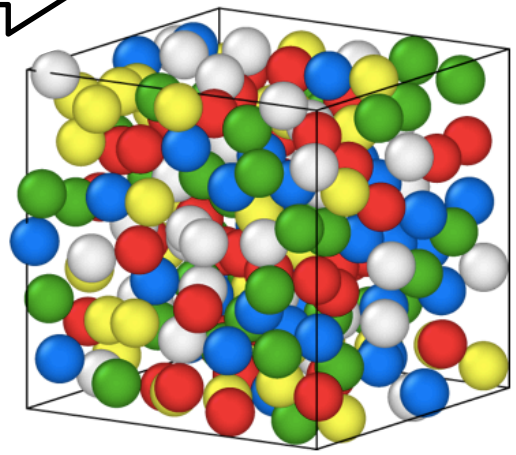




PARADIGM SHIFT

GLASS





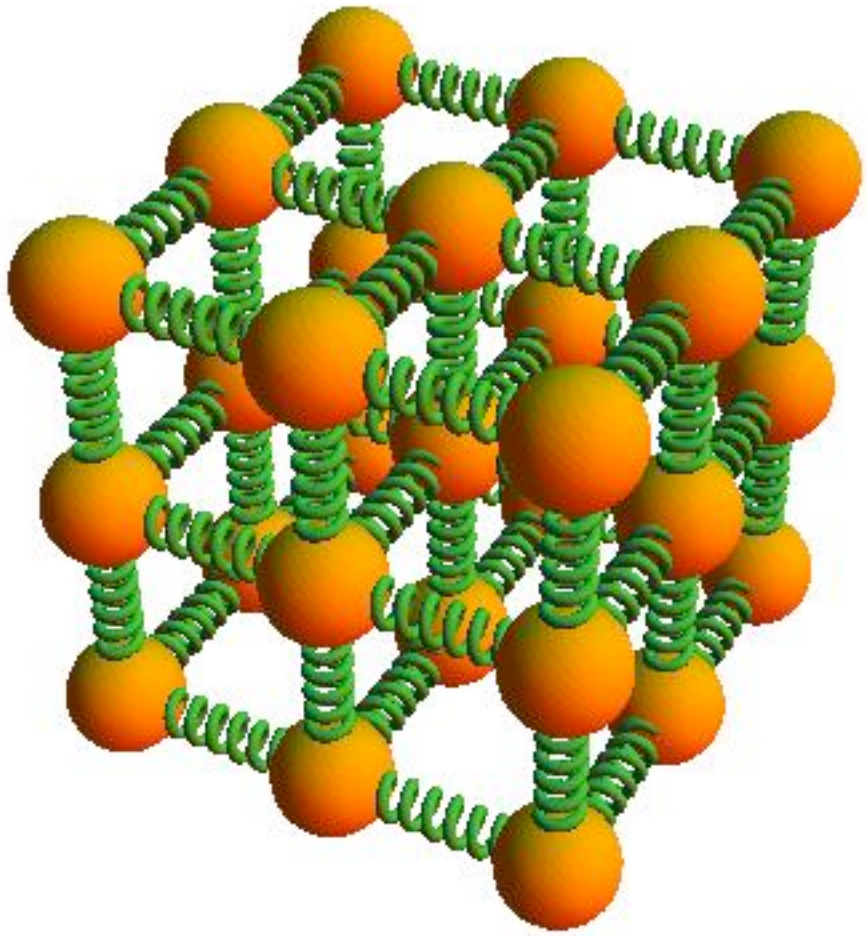
GLASSCOTT NAT. COMM. 2019

....

VIBRATIONAL PROPERTIES

VIBRATION OF CONFIG. AROUND MINIMA

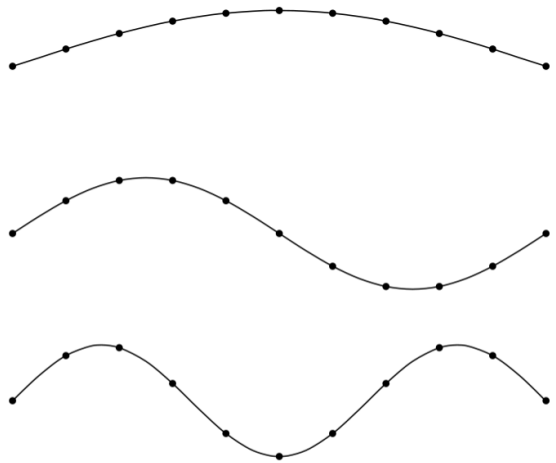
CRYSTALS, PERIODIC LATTICE:

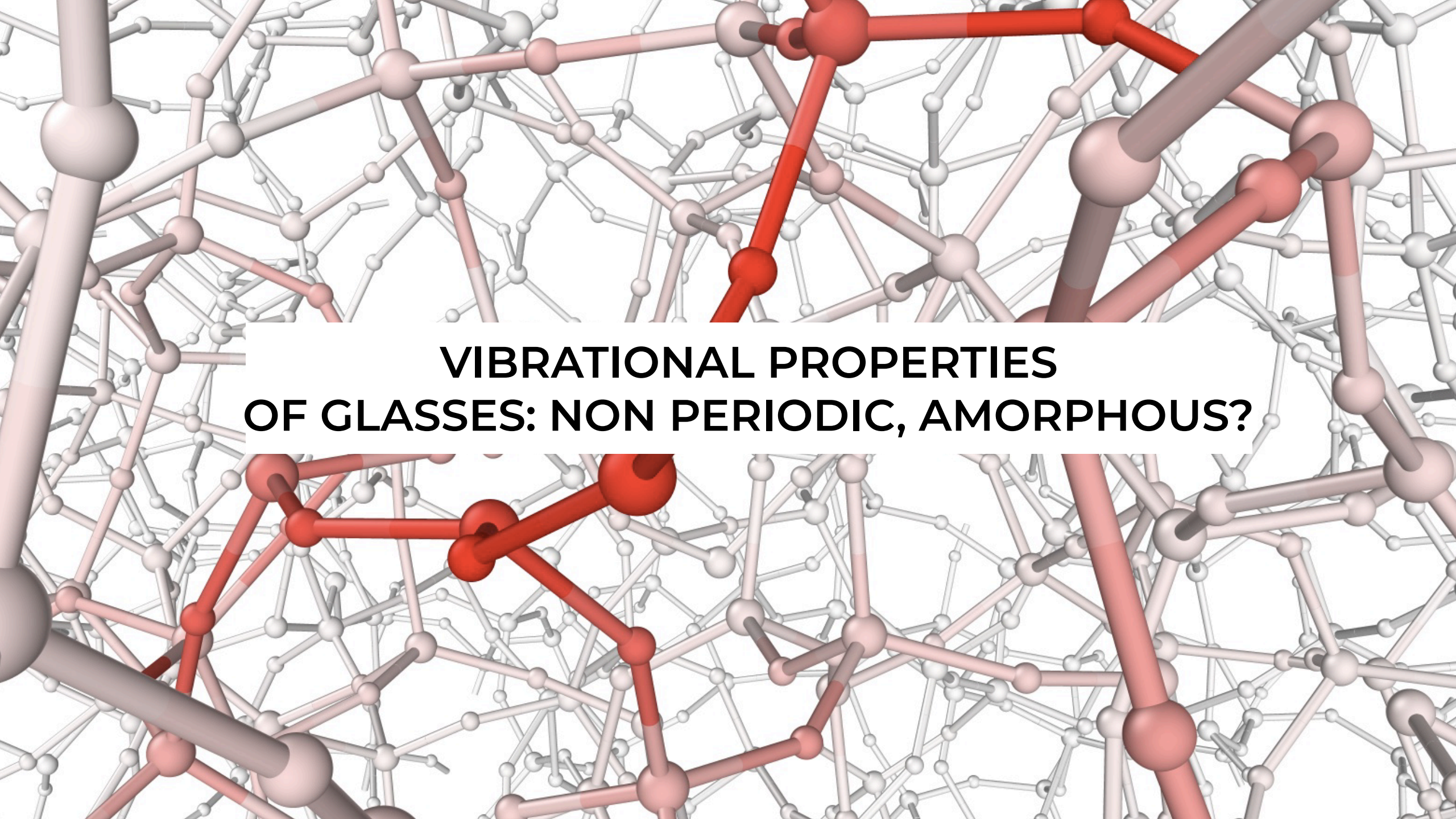


DEBYE'S THEORY PREDICTS

$$D(\omega) \propto \omega^{d-1}$$

"EXTENDED" PHONON MODES





VIBRATIONAL PROPERTIES OF GLASSES: NON PERIODIC, AMORPHOUS?

RECENT NUMERICAL STUDIES

$$D(\omega) = A\omega^{d-1} + B\omega^4$$

PHONON MODES PREDICTED BY THE DEBYE THEORY

NON-PHONON MODES ORIGINATE FROM GLASSY CONFIGURATION

LERNER, DURING, AND BOUCHBINDER, PRL 2016

MIZUNO, SHIBA, AND IKEDA, PNAS 2017

LERNER, AND BOUCHBINDER, J. CHEM. PHYS. 2021

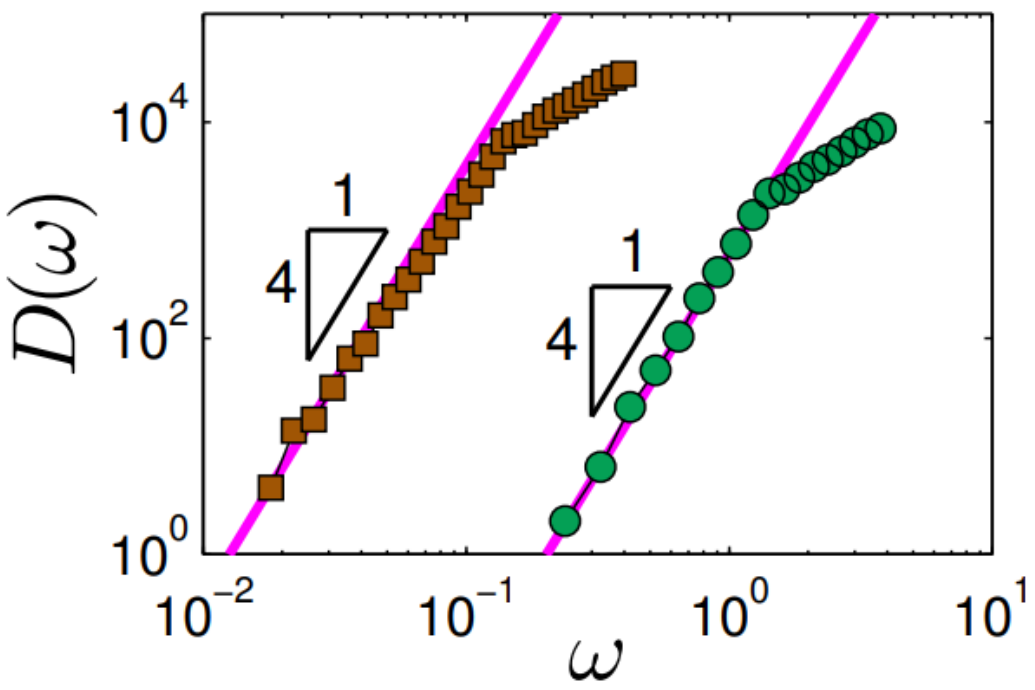
HYBRIDIZATION OF MODES!

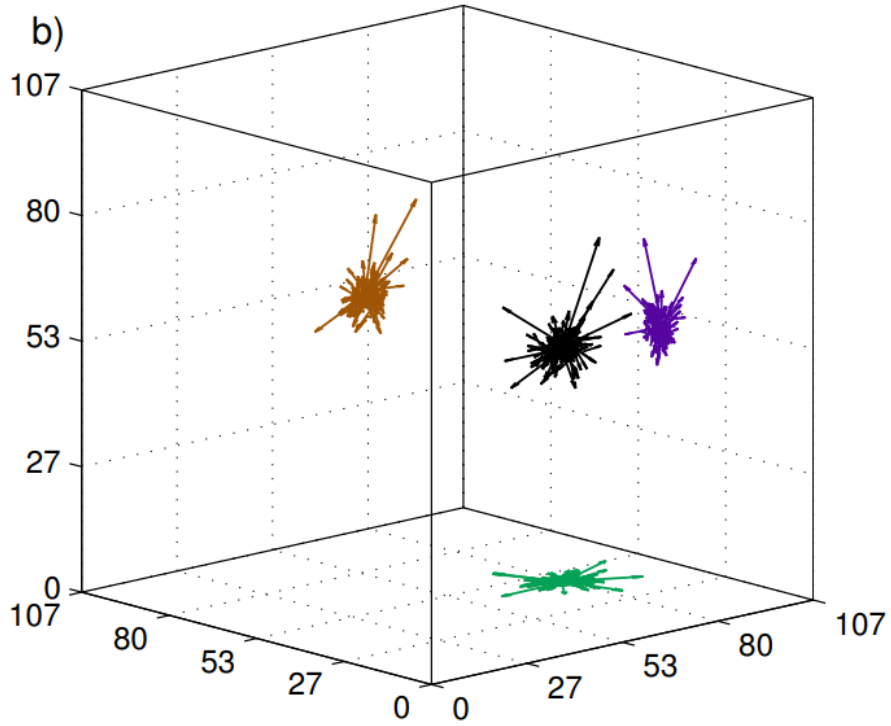
HOW TO DISENTANGLE PHONON MODES AND NON-PHONON MODES?

RECENT NUMERICAL STUDIES

LERNER, DURING, AND BOUCHBINDER, PRL 2016

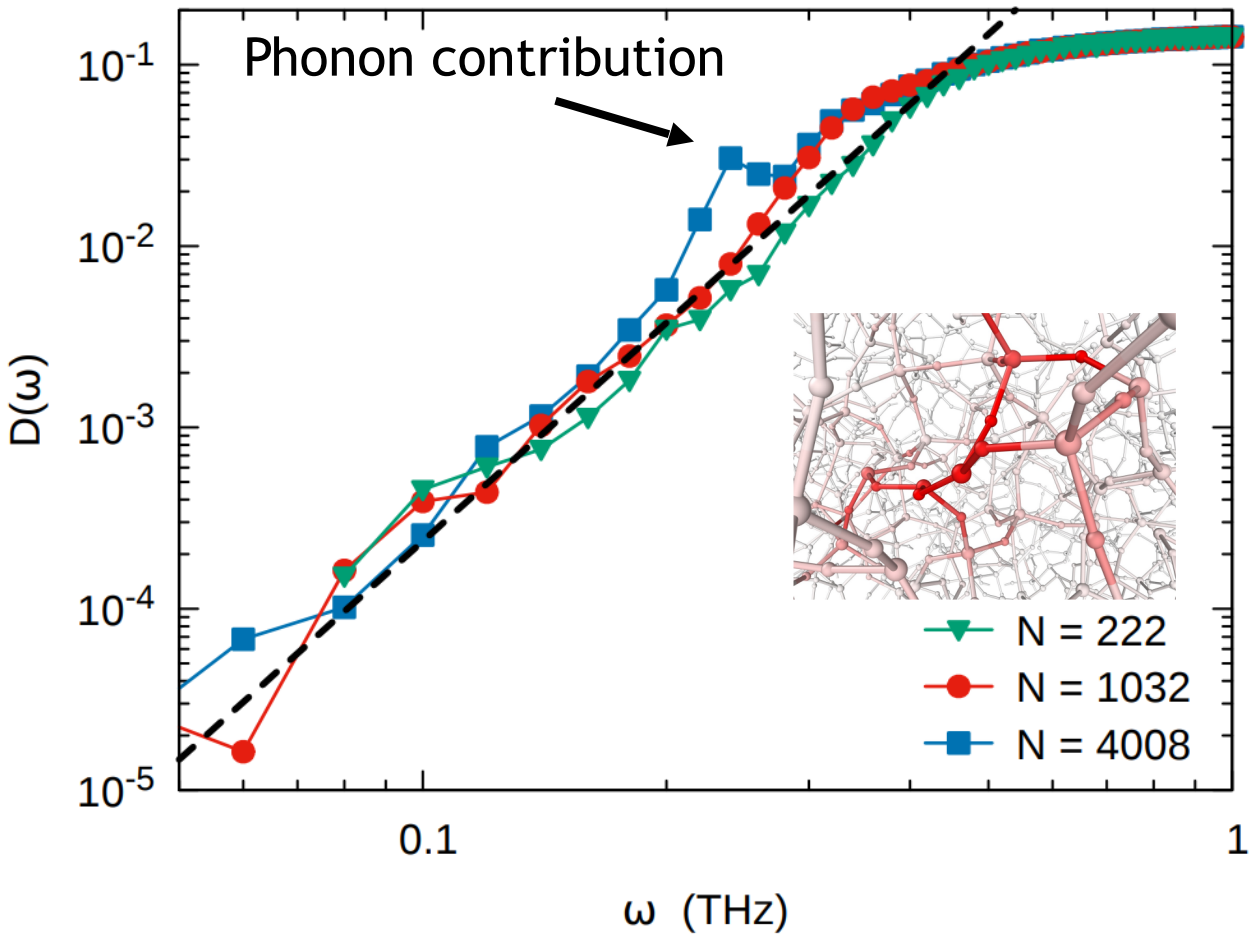
THE LOWEST PHONON MODE SCALES WITH L^{-1}





THE NON-PHONON MODES ARE MAINLY OBSERVED IN SIMPLE POTENTIAL SYSTEMS.
REALISTIC MODELS?

THE CASE OF SILICA GLASS



WE NUMERICALLY CONFIRMED $D(\omega) \propto \omega^4$

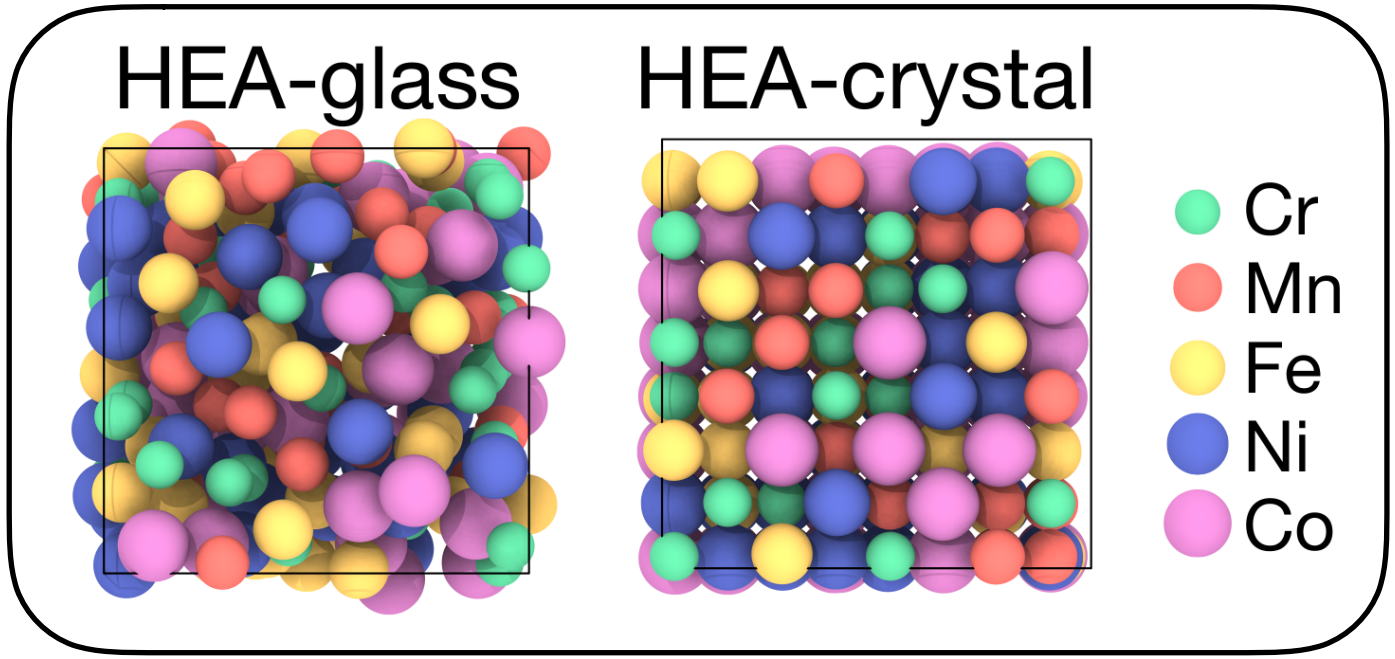
BONFANTI, GUERRA, MONDAL, PROCACCIA, & ZAPPERI, PRL 2020

THE CASE OF HEAS
WHAT IS THE ROLE OF [COMPOSITIONAL] DISORDER?

THE CASE OF HEAS
WHAT IS THE ROLE OF [COMPOSITIONAL] DISORDER?

Model of disordered binary alloys:
Lerner, and Bouchbinder, PRL 2022

THE CASE OF HEAS
WHAT IS THE ROLE OF [COMPOSITIONAL] DISORDER?

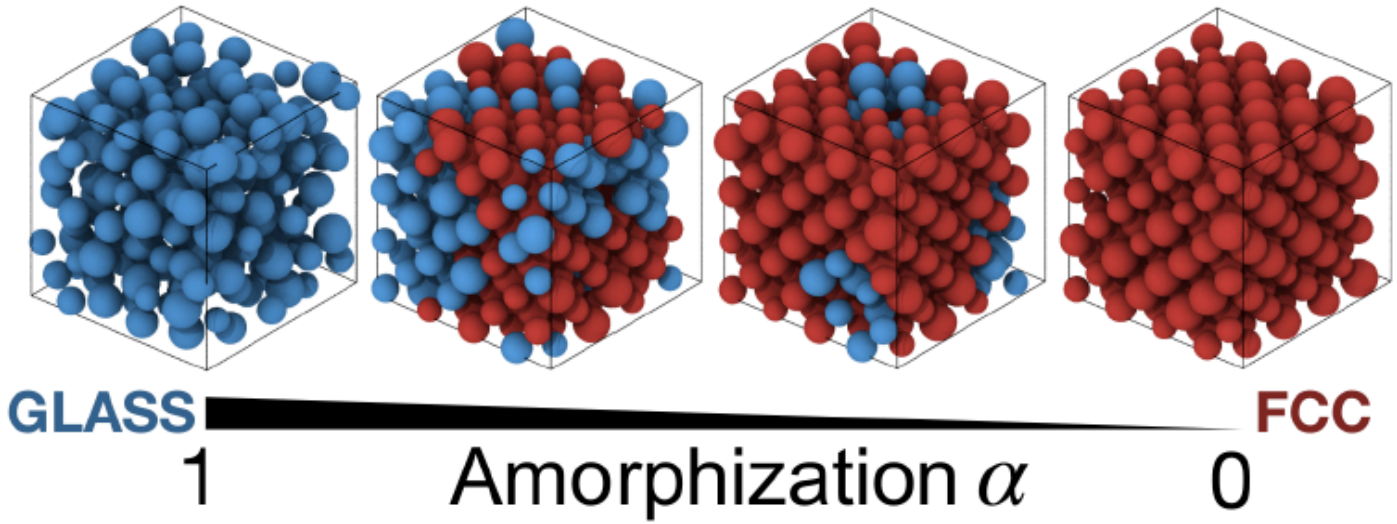


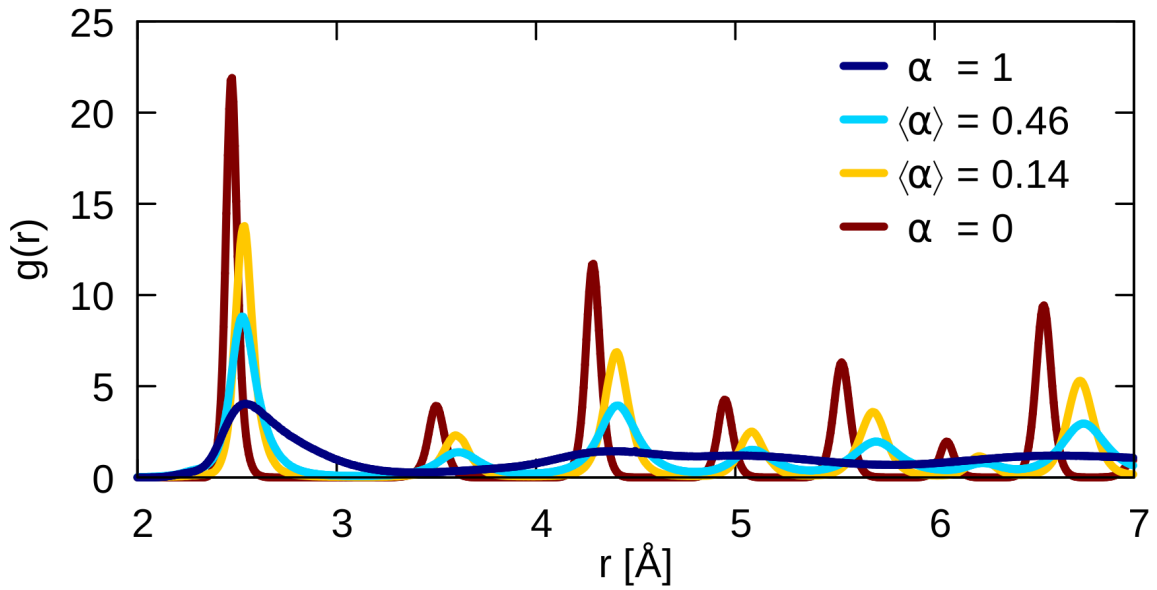
- CANTOR ALLOY
- REALISTIC POTENTIAL APPROPRIATE FOR METALLIC SYSTEMS: EAM POTENTIAL
- SMALL SYSTEM SIZE ~ 250 ATOMS
- VIBRATIONAL MODES CALCULATION:

$$H_{ij}^{\alpha\beta} \equiv \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 U(\boldsymbol{r}_1, \cdots \boldsymbol{r}_N)}{\partial r_i^\alpha \partial r_j^\beta}$$

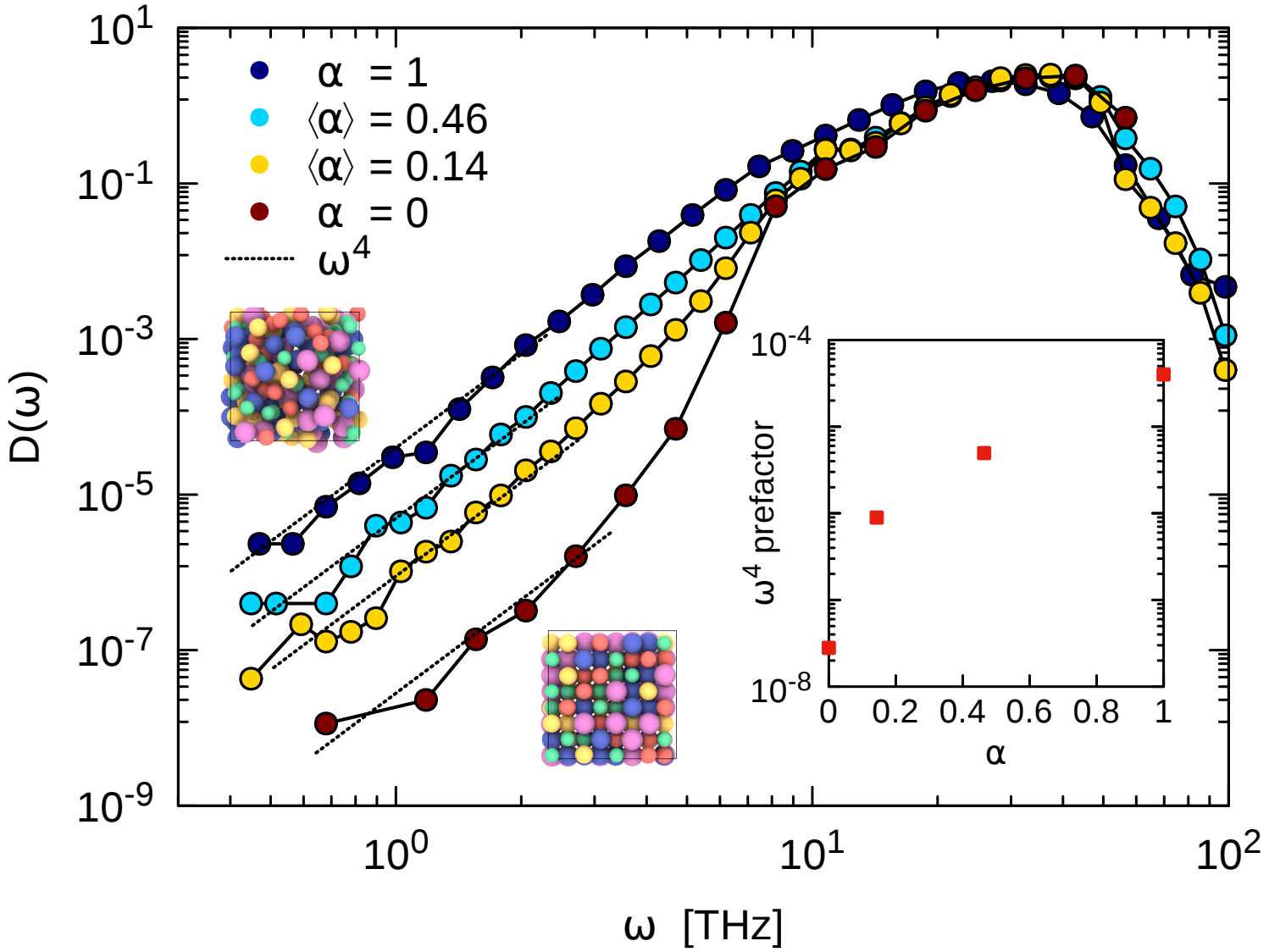
ROLE OF DISORDER

$$\alpha = 1 - \frac{N_{FCC}}{N}$$

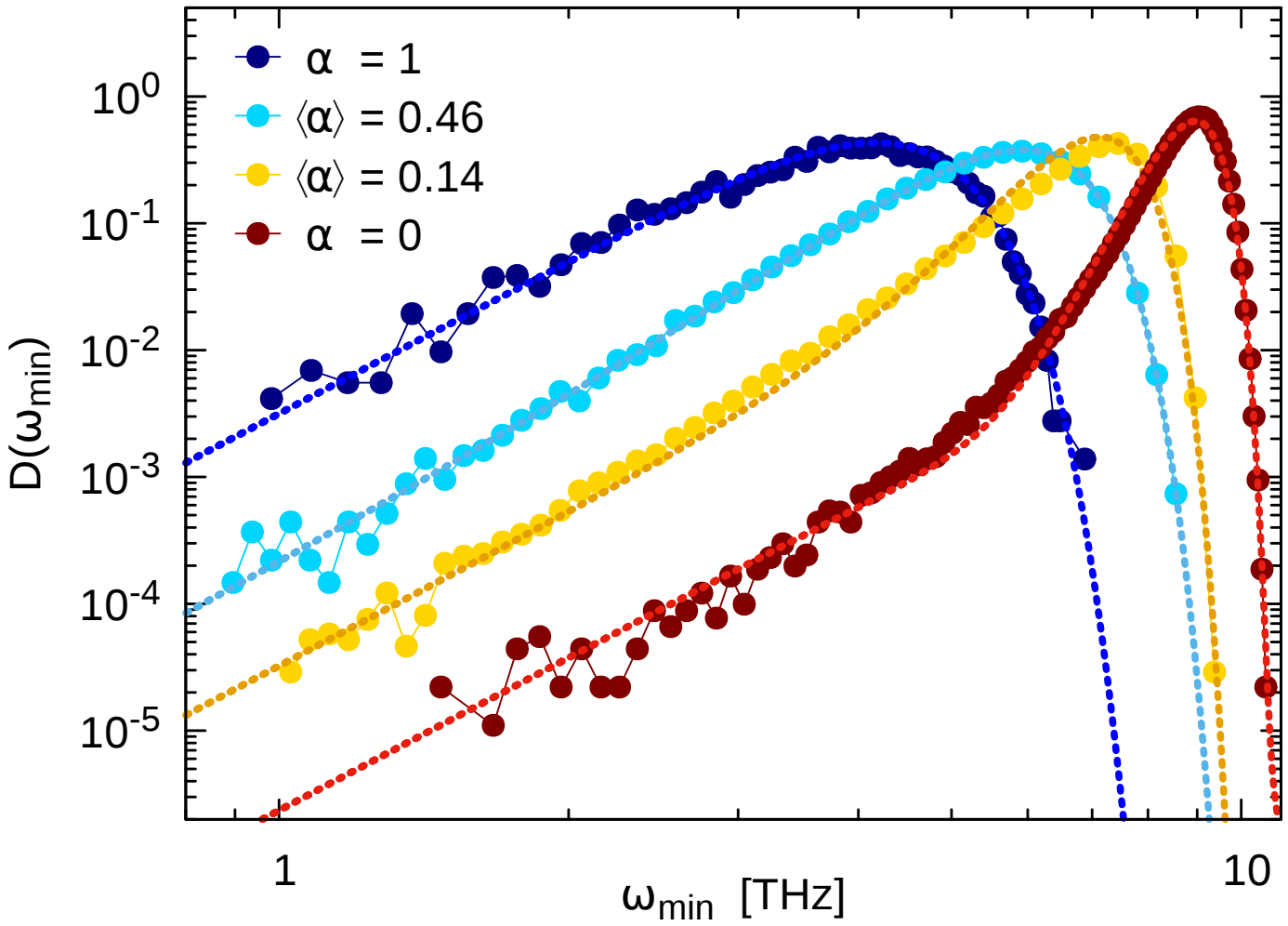




DOS of High Entropy Alloys (HEA) follow ω^4 **also** in crystal structures

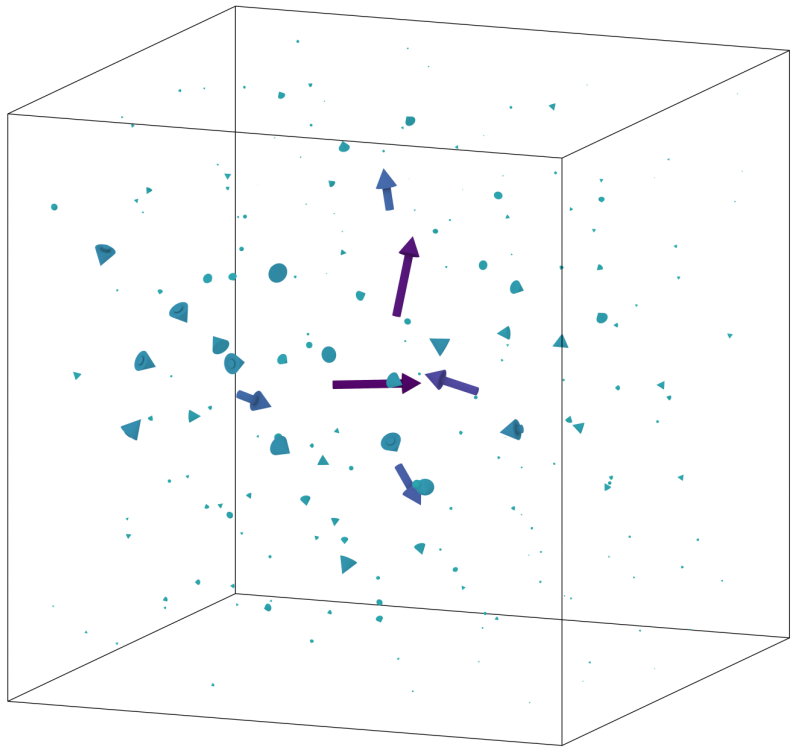


MINIMUM EIGENFREQUENCY

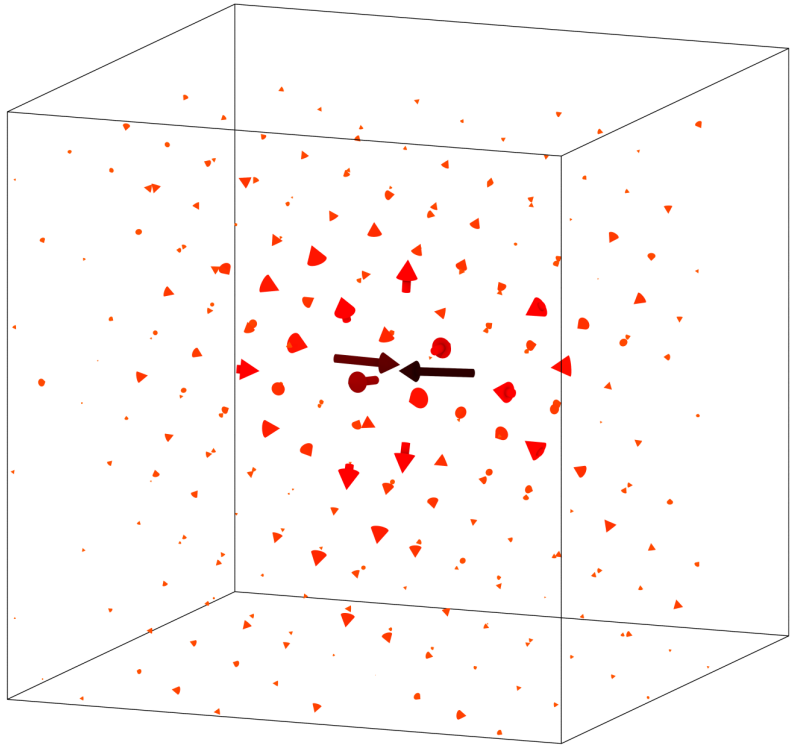


Distribution of ω_{min} follows Weibull

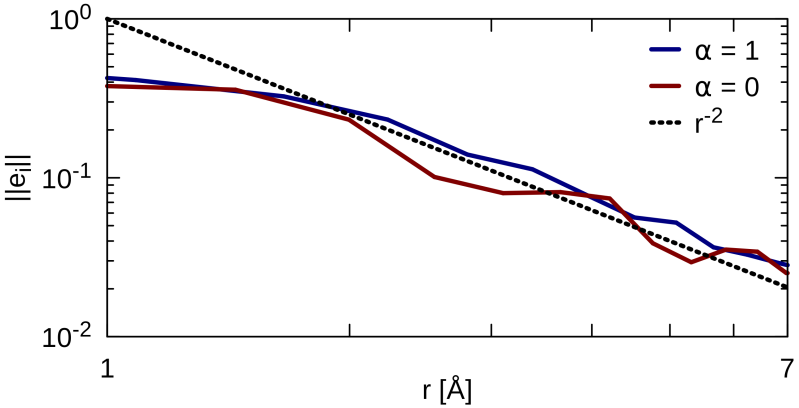
MODES ARE LOCALIZED



HEA-GLASS



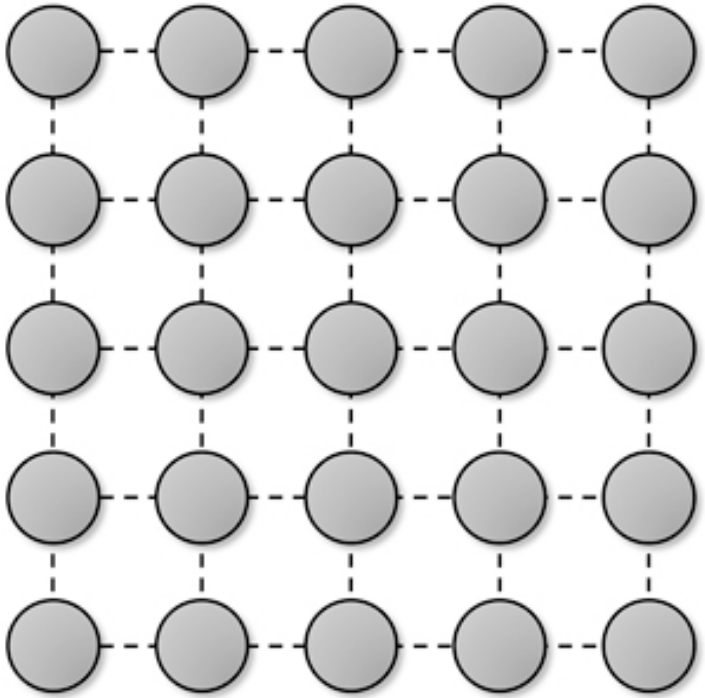
HEA-CRYSTAL



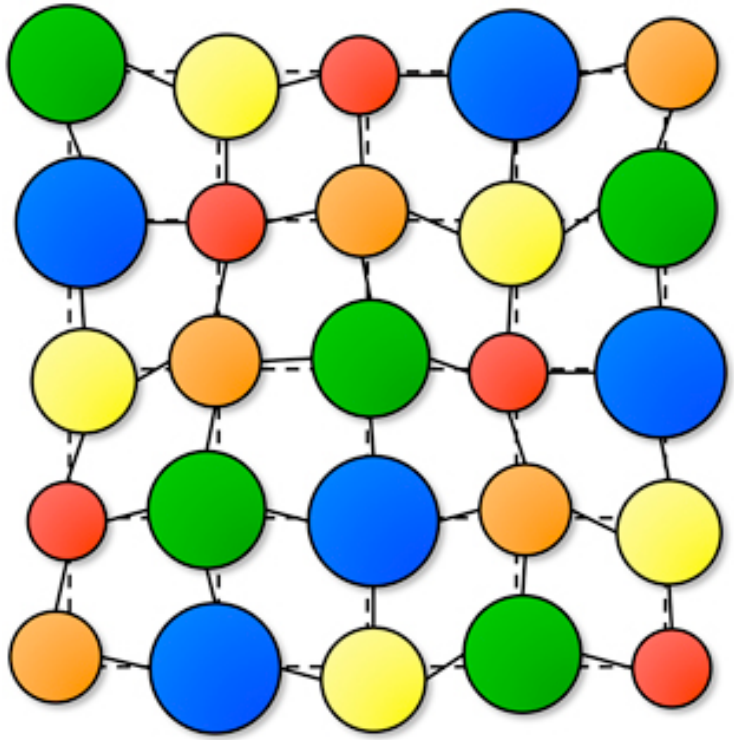
Long range trend

LATTICE DISTORSION

CONVENTIONAL ALLOYS



CRYSTALLINE HEAS



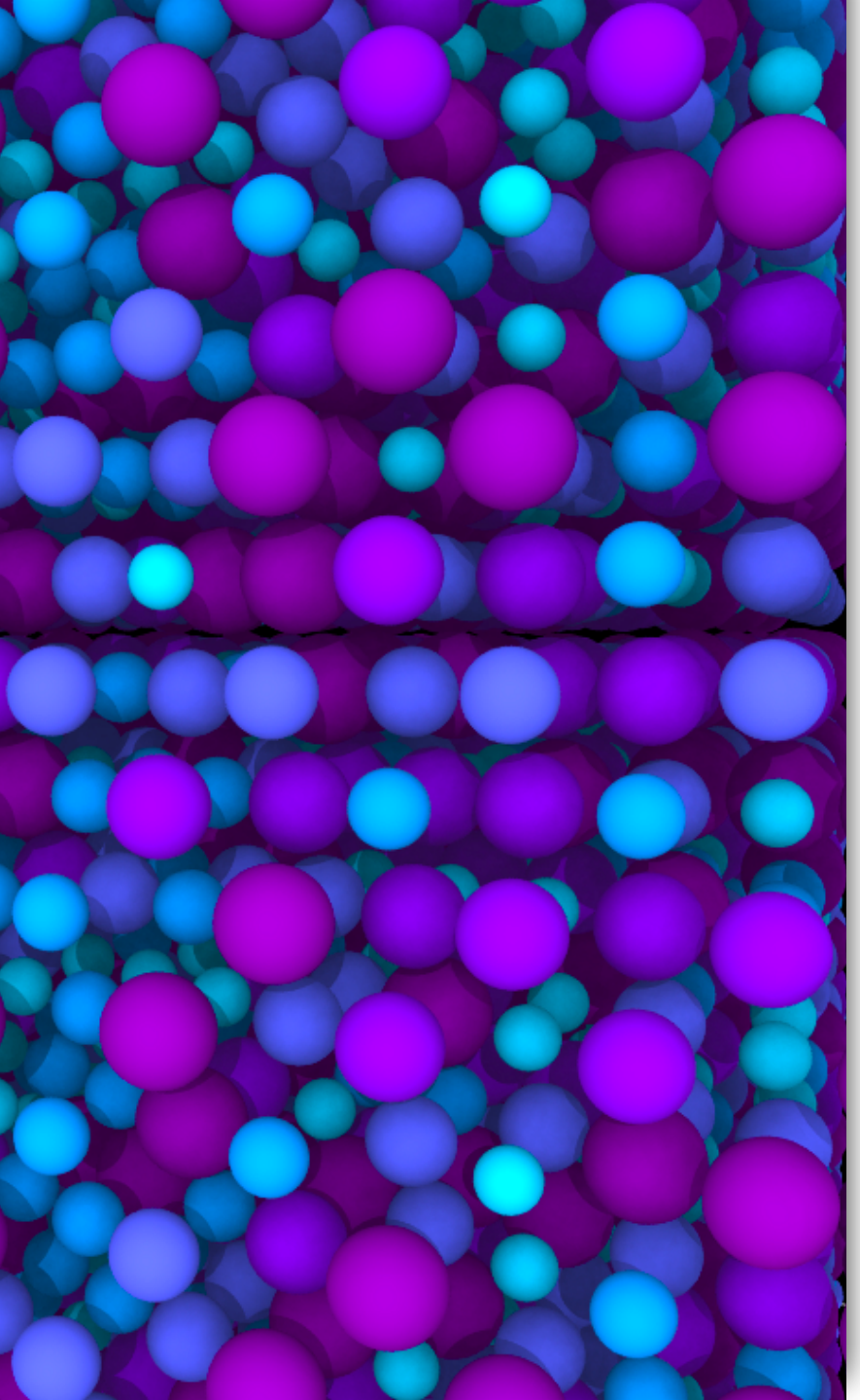
[Submitted on 16 Mar 2023]

Quasi-localized modes in crystalline high entropy alloys

Silvia Bonfanti, Roberto Guerra, Rene Alvarez-Donado, Pawel Sobkowicz, Stefano Zapperi, Mikko Alava

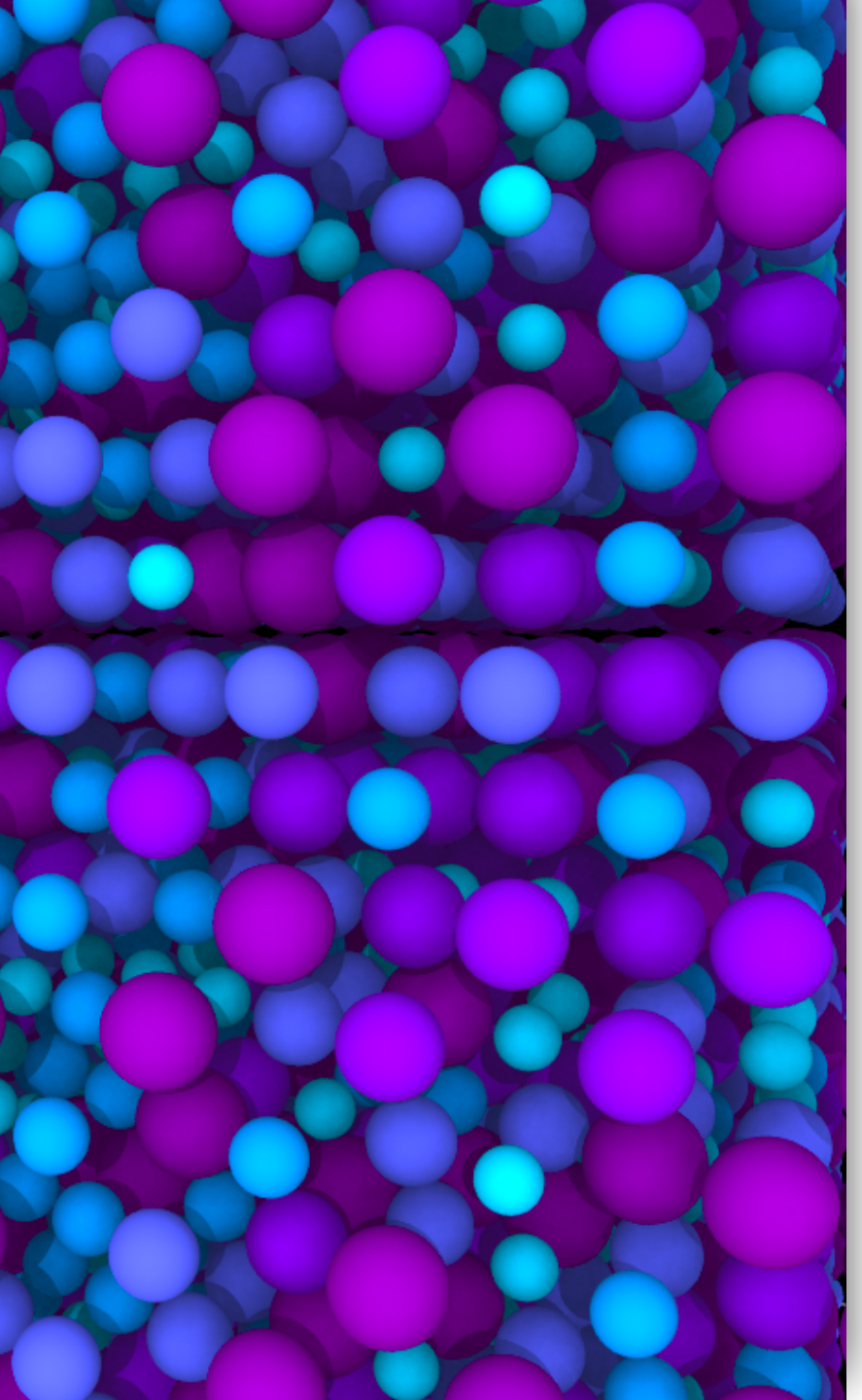
High Entropy Alloys (HEAs) are designed by mixing multiple metallic species in nearly the same amount to obtain crystalline or amorphous materials with exceptional mechanical properties. Here we use molecular dynamics simulations to investigate the role of positional and compositional disorder in determining the low-frequency vibrational properties of CrMnFeCoNi HEAs. Our results show that the expected dependence of the density of states on the frequency as $D(\omega) \sim \omega^4$ is recovered for amorphous HEAs and is also observed for partially crystallized alloys with deviations that depend on the degree of crystallization. We find that the quasi-localized vibrations are still visible in crystalline HEAs, albeit suppressed compared to the corresponding amorphous alloys. Our work offers a unified perspective to describe HEA mechanical properties in terms of their vibrational density of states.

Comments: 8 pages, 7 figures
Subjects: **Disordered Systems and Neural Networks (cond-mat.dis-nn)**; Materials Science (cond-mat.mtrl-sci)
Cite as: arXiv:2303.09161 **[cond-mat.dis-nn]**
(or arXiv:2303.09161v1 **[cond-mat.dis-nn]** for this version)
https://doi.org/10.48550/arXiv.2303.09161



FUTURE PERSPECTIVES

- CAN WE INDIRECTLY SPOT QLM IN EXPERIMENTS IN HEAS?
- RELATION WITH THE MECHANICAL PROPERTIES
  - LOW-FREQUENCY ENERGY BARRIERS TAKE PLACE WHERE THE MATERIAL BREAKS. HEAS?



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