



IChF

HZB Helmholtz
Zentrum Berlin

Detection of vacancies in FCC solid and their effect on twinning

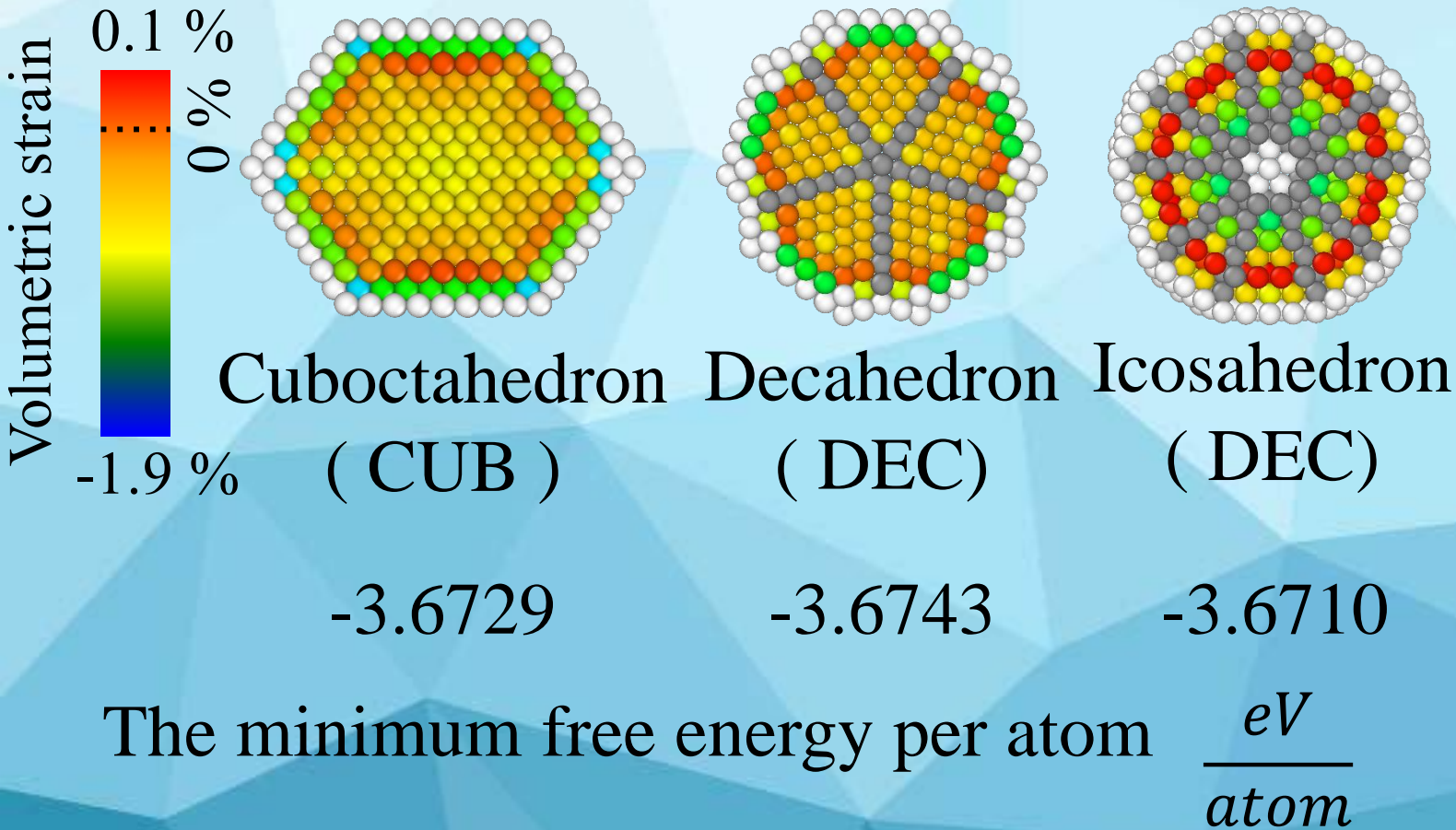
Ilia Smirnov ^a, Zbigniew Kaszukur ^a, Armin Hoell ^b

^a - Institute of Physical Chemistry, Warsaw, Poland

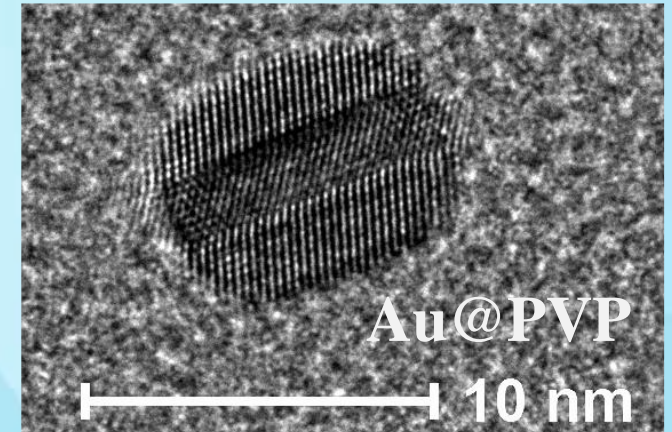
^b - Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

ISSRNS Cracow, August 22, 2022

What is the most stable form of FCC nano crystals?

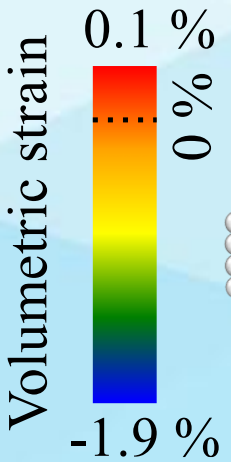
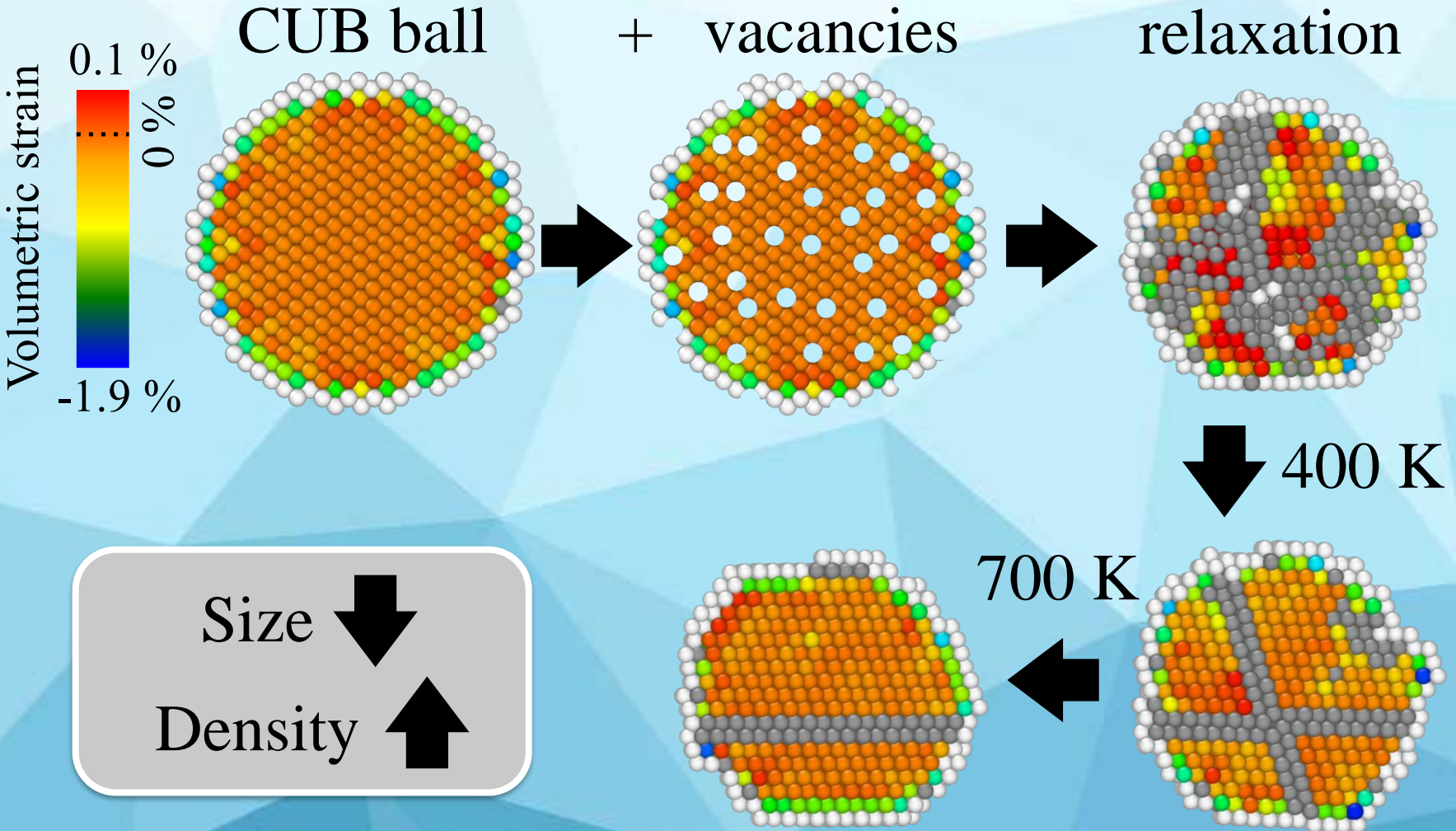


Are there other forms?



What mechanism triggers the twinning ?

How do vacancies affect twinning ?



● twin plane atoms / vacancy neighbor

Models were visualized in OVITO

Size ↓
Density ↑

All calculations were done by CLUSTER.

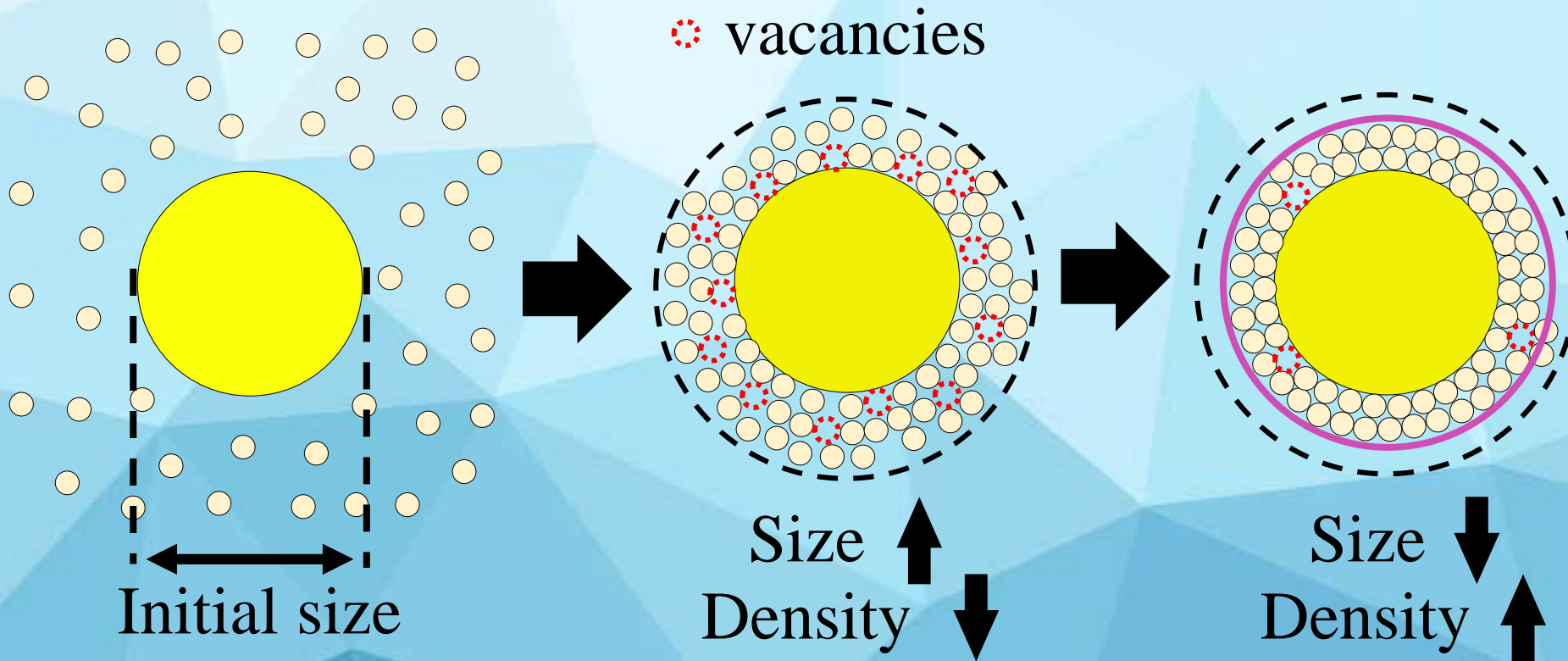
Initial **ISOLATED** computational model (top => bottom)

Where do vacancies come from?



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Ostwald ripening / condensation of atoms



How to detect these key parameters?

TEM
XRD
SAXS

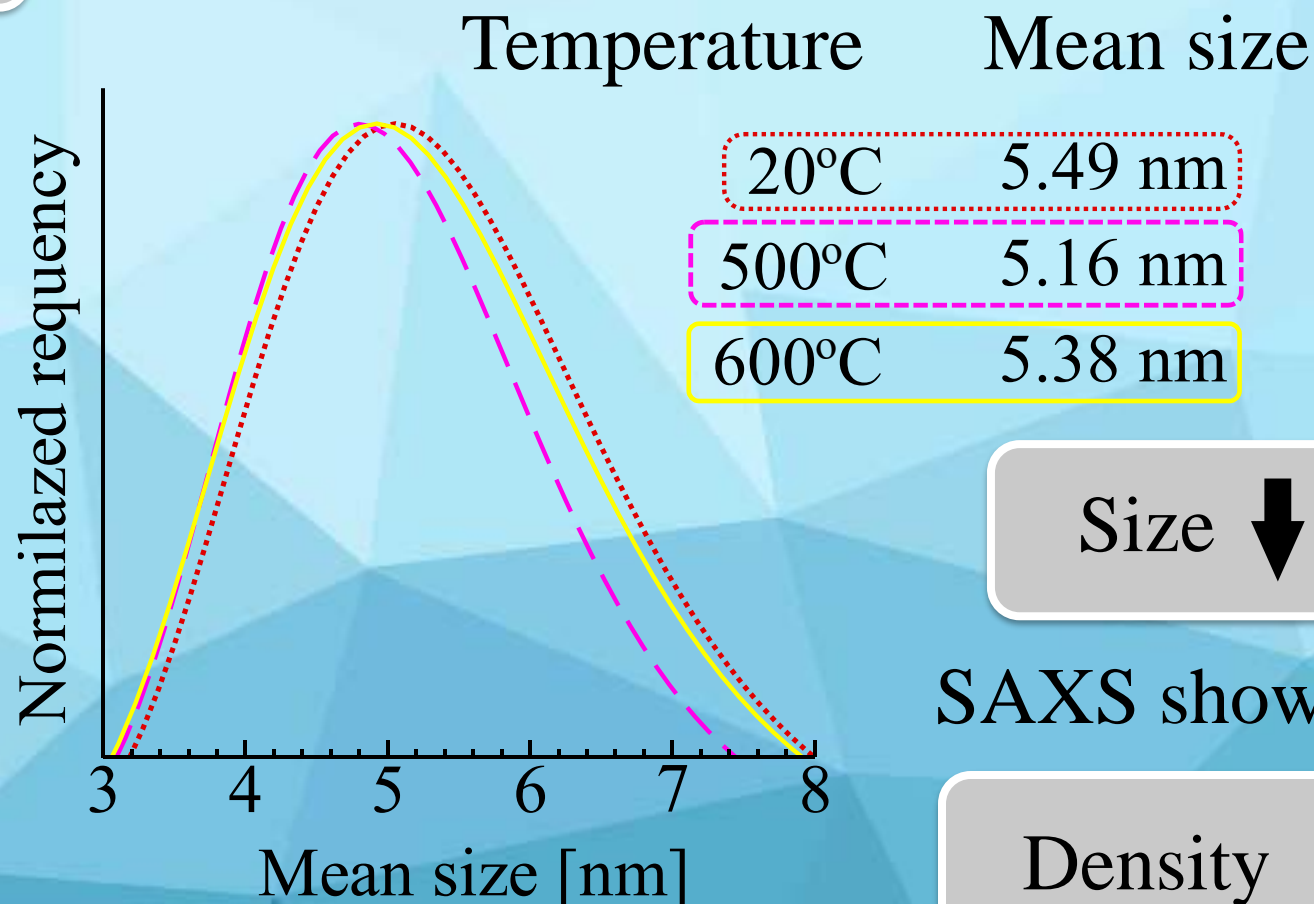
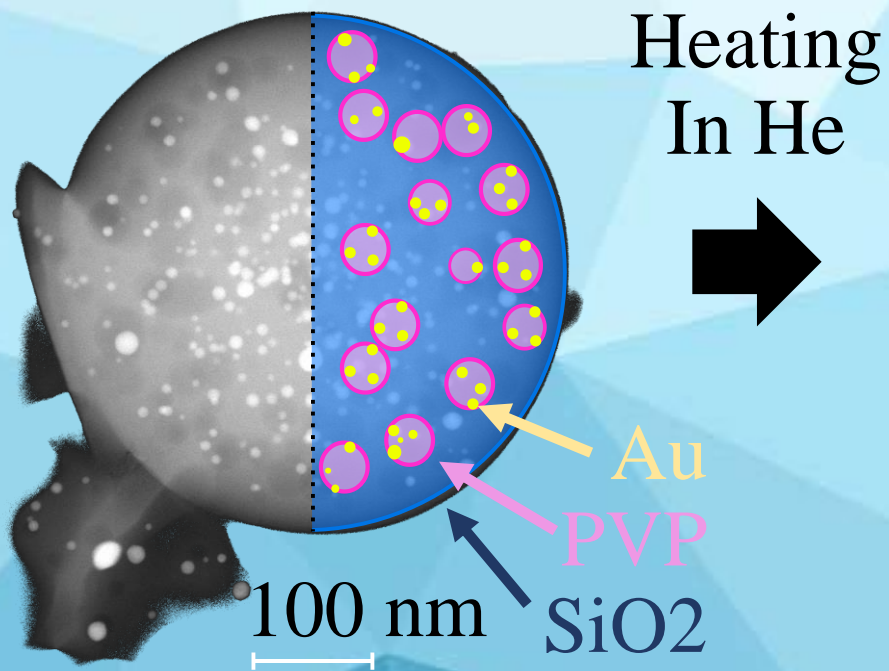
If there are such changes -> the vacancies is confirmed (?)

TEM “observation” of vacancies



Au NPs encapsulated in SiO₂

Number weighted size distribution (TEM)



Size ↓

SAXS shows

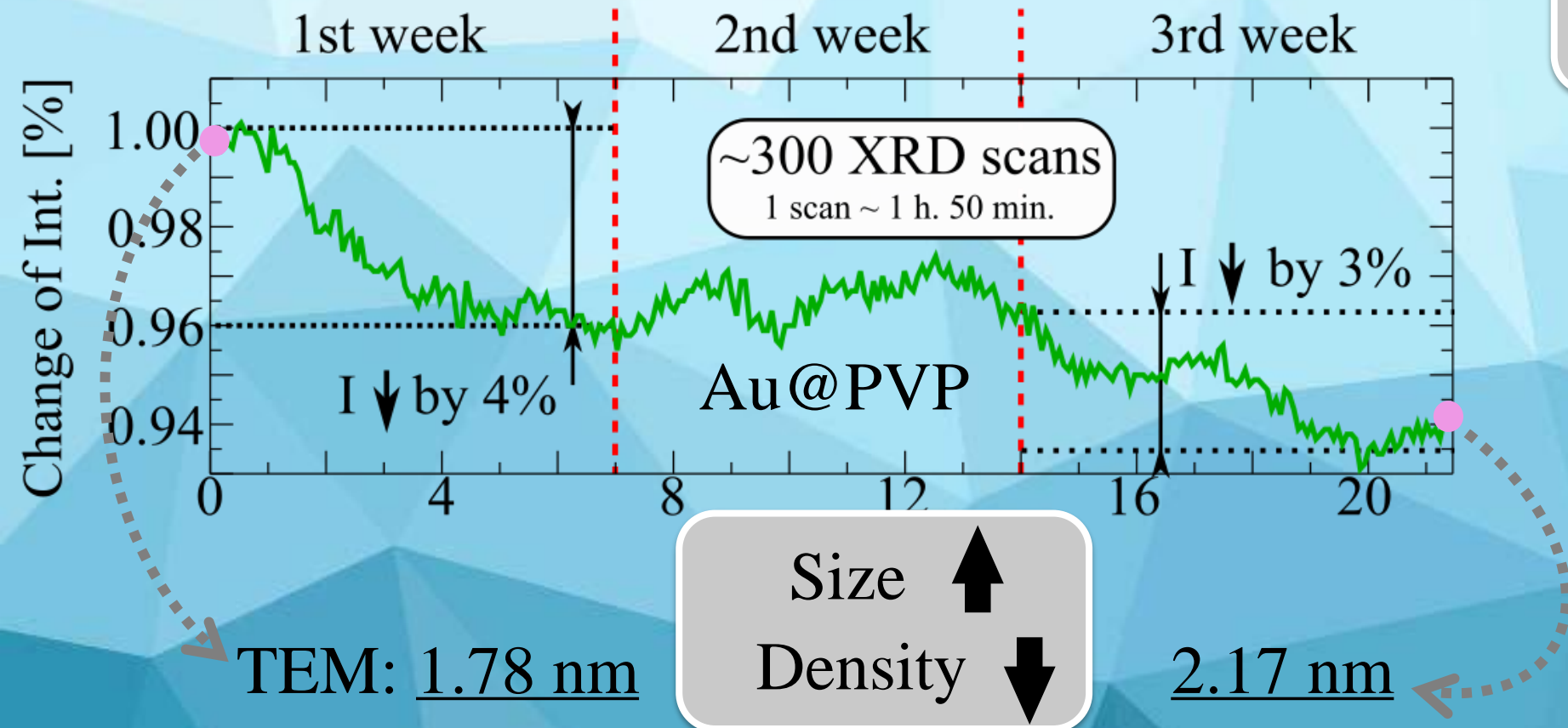
Density ↑

XRD “observation” of vacancies



FCC metals evolve under exposure to Cu X-rays

Is it typical for all FCC metals ?



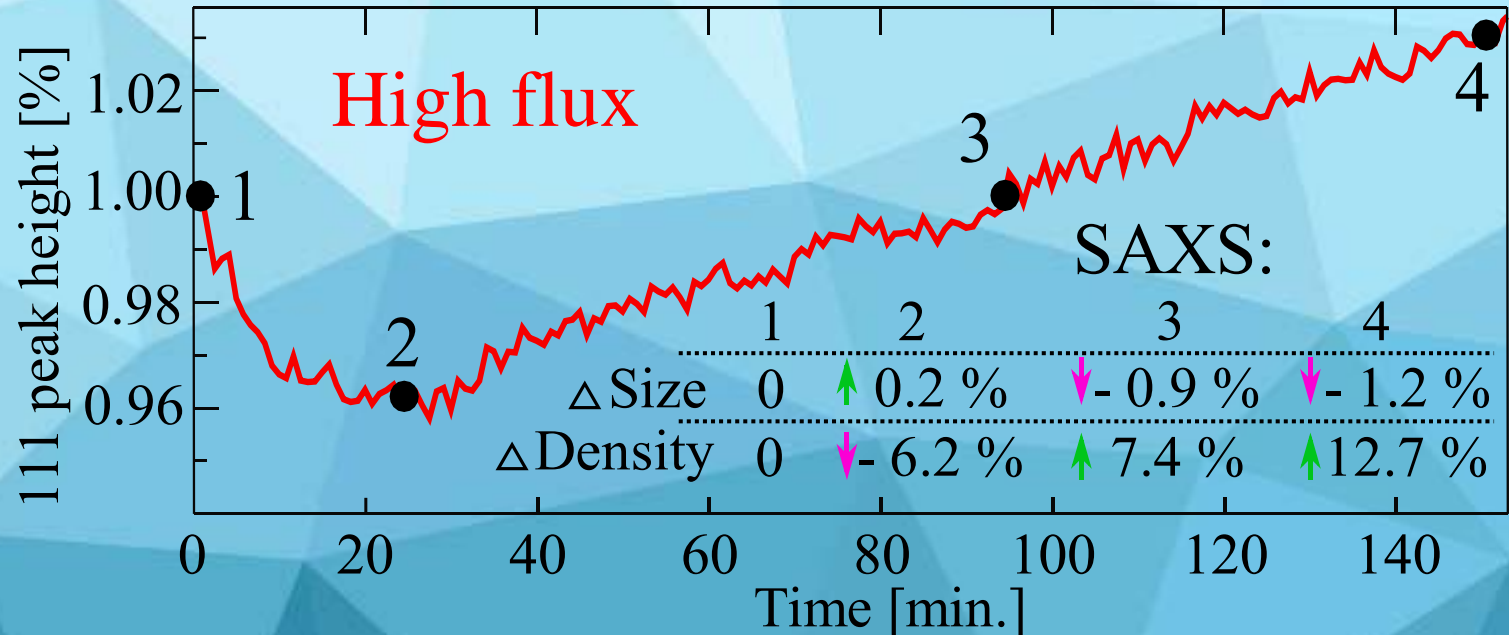
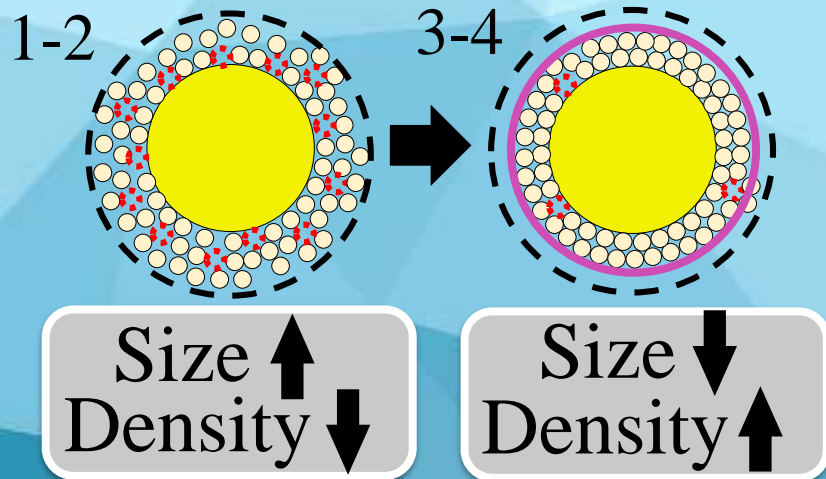
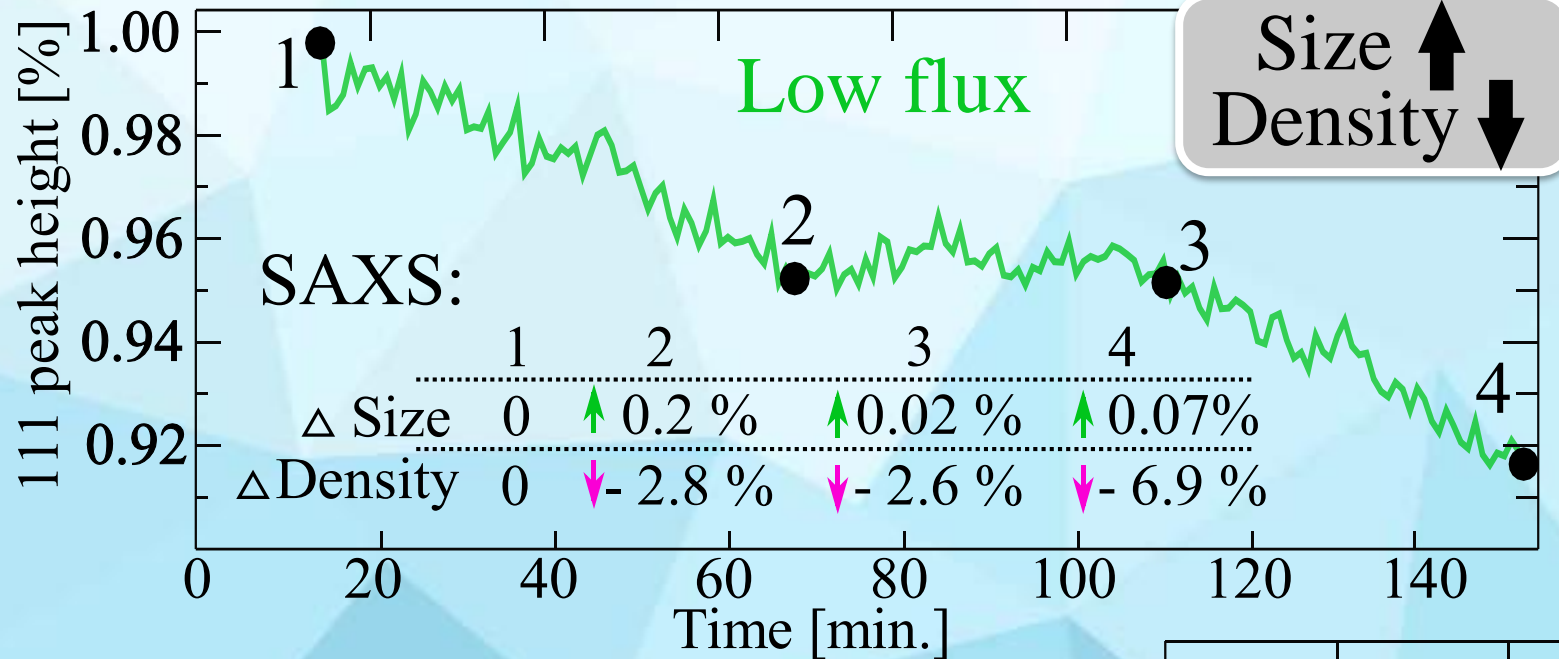
It is typical for:
Cu, Ir, Pt, Ni, and
Au (macrocrystals
were also tested)

In-situ SAXS + WAXS



Au@PVP (1.78 nm)

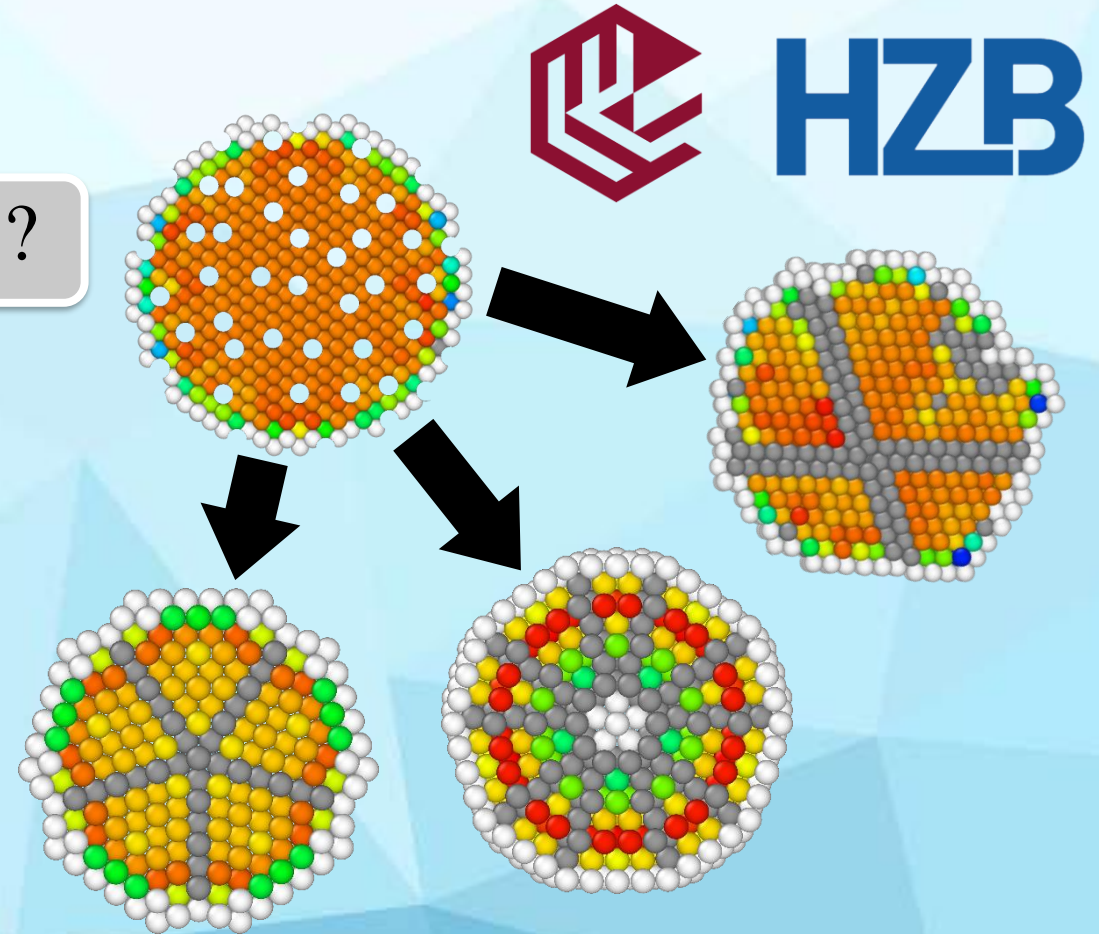
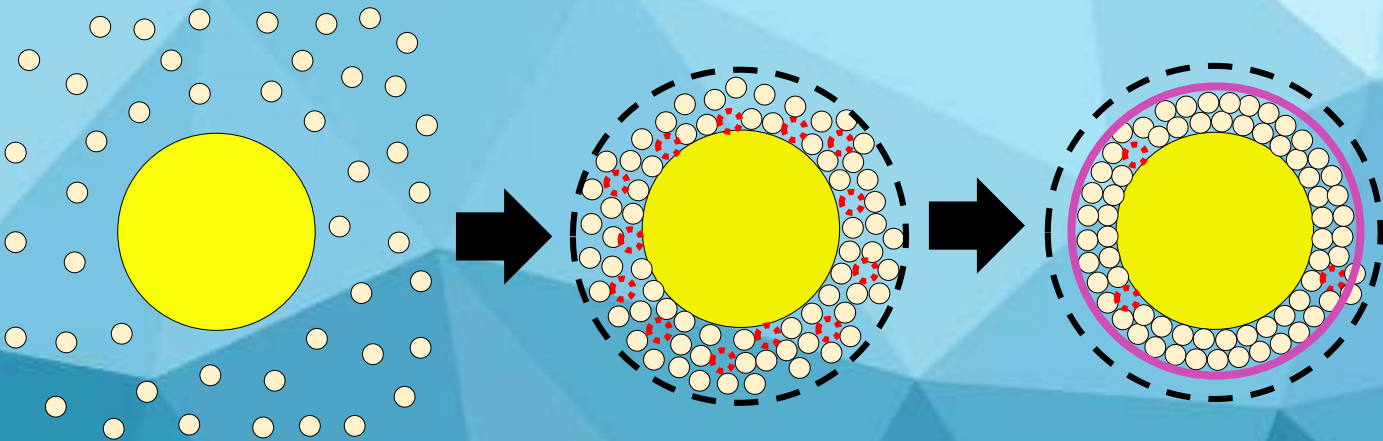
DESY, Hamburg
Beamline PS 62



Conclusions:

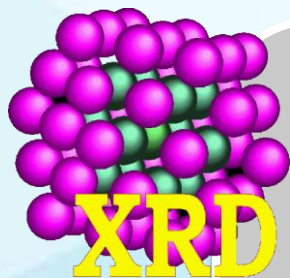
How do vacancies affect twinning ?

- 1) To verify vacancies driven twinning we need to detect vacancies
- 2) Only depend parameters can be measured: density and size of particles



- 3) Theoretical predictions were confirmed by three independent techniques

Acknowledgments :



Members of XRD Group

ICHF, Warsaw

Wojciech Juszczyk, PhD
Bogusław Mierzwa, PhD
Dmytro Lisovytskiy, PhD



Dr. Sylvio Haas (DESY,
beamline P62 responsible,
Hamburg)

We thank DESY for
supplying beamtime for
this project under proposal
number: I-20210744 EC.

Ph.D. Marion Flatken
(Helmholtz-Zentrum
Berlin)

Thank you for your attention!