



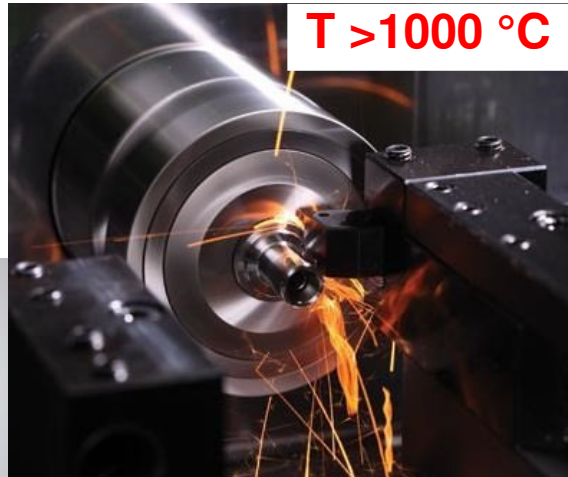
Learning hardness

Ferenc Tasnádi, H. Levämäki, R. Armiento and I.A. Abrikosov

2021-05-24

Motivation - Coating industry

“More” machining:

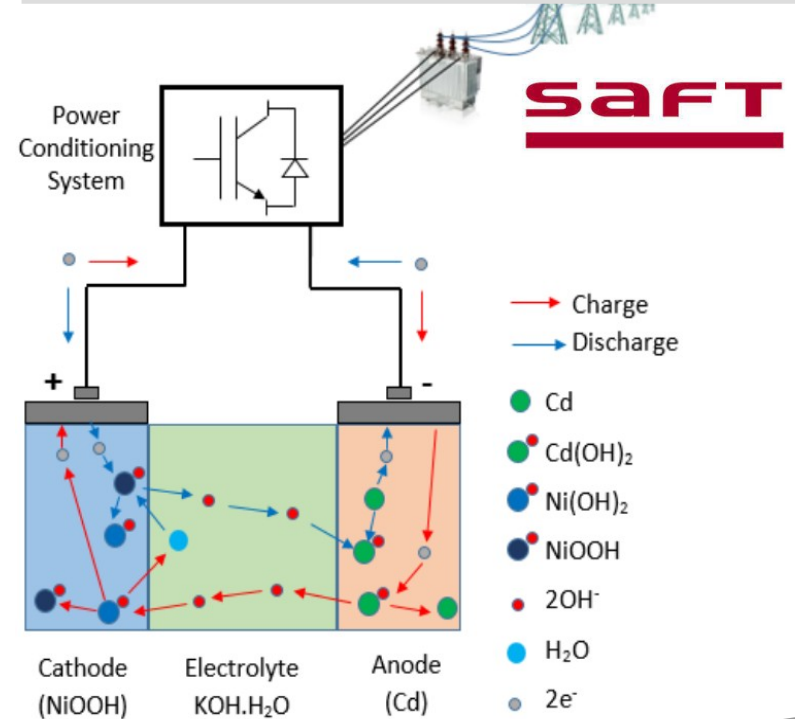


ionbond
THE SURFACE ENGINEERS™
PVD, CVD, and PACVD Coating Technology

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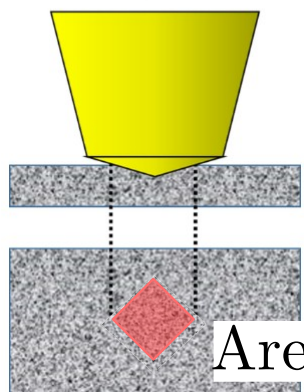
Electrochemical performance:



Measured H vs. E^* of complex nitrides

Micromechanical testing:
indentation

Load: 50-150 mN

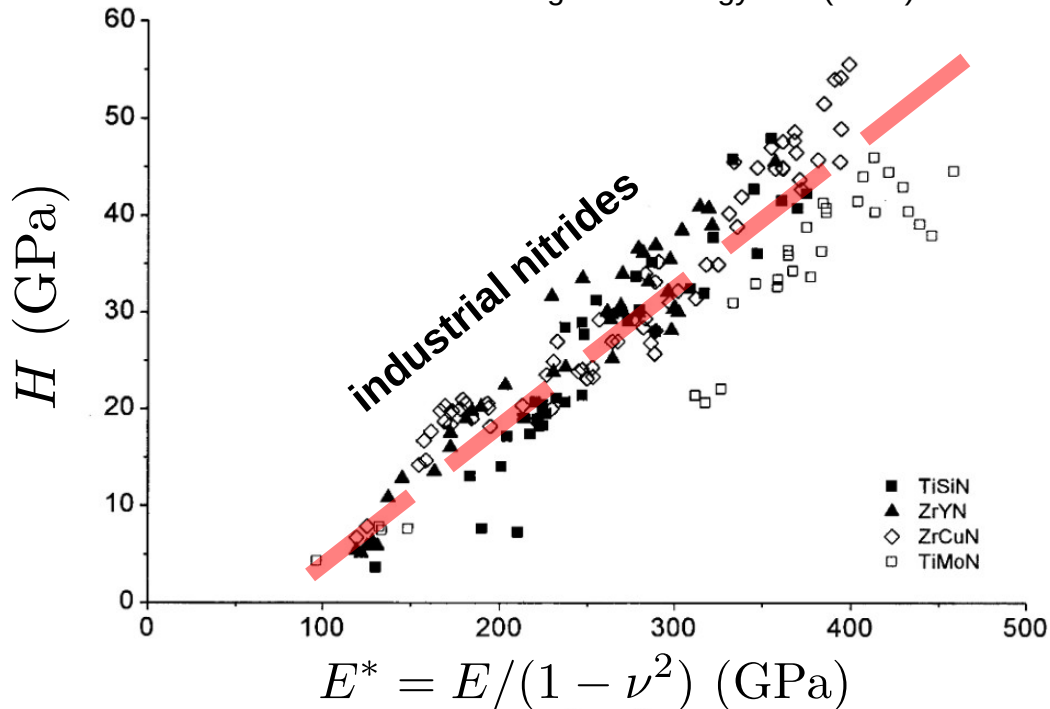


$$H = \frac{L}{A} \text{ (GPa)}$$

$$E^* = \frac{1}{2} \sqrt{\frac{\pi}{A}} S \text{ (GPa)}$$

Area (μm)²

Surface and Coatings Technology 154 (2002) 304



E : Young's modulus

S : slope of initial unload

ν : Poisson ratio

Elastic constants of disordered nitrides

Materials Project
<https://next-gen.materialsproject.org/>

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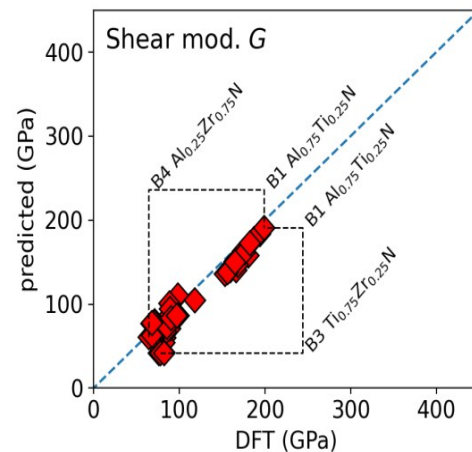
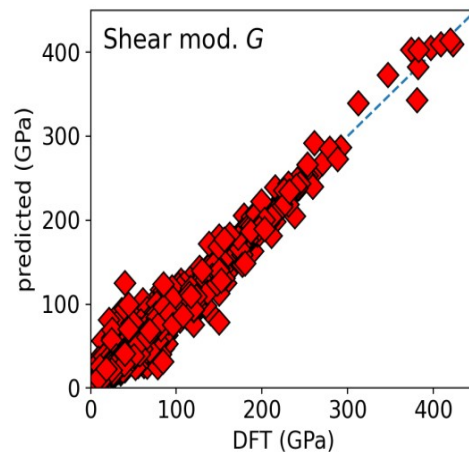
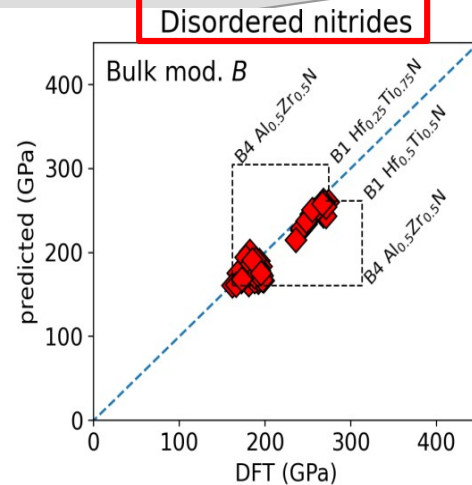
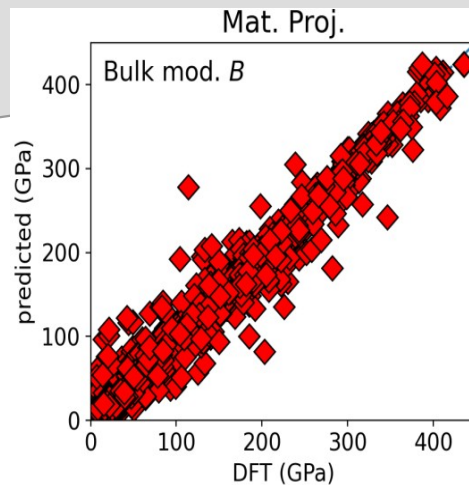
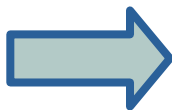
- chemical elements
- composition
- crystal structure (B1, B3, B4)

Labels:

- total energy
- stress tensor
- forces
- elastic tensor
- Bulk modulus
- Shear modulus

≈ 8000 labeled data

crystal graph convolutional neural network (CGCNN)



Elastic constants of disordered nitrides

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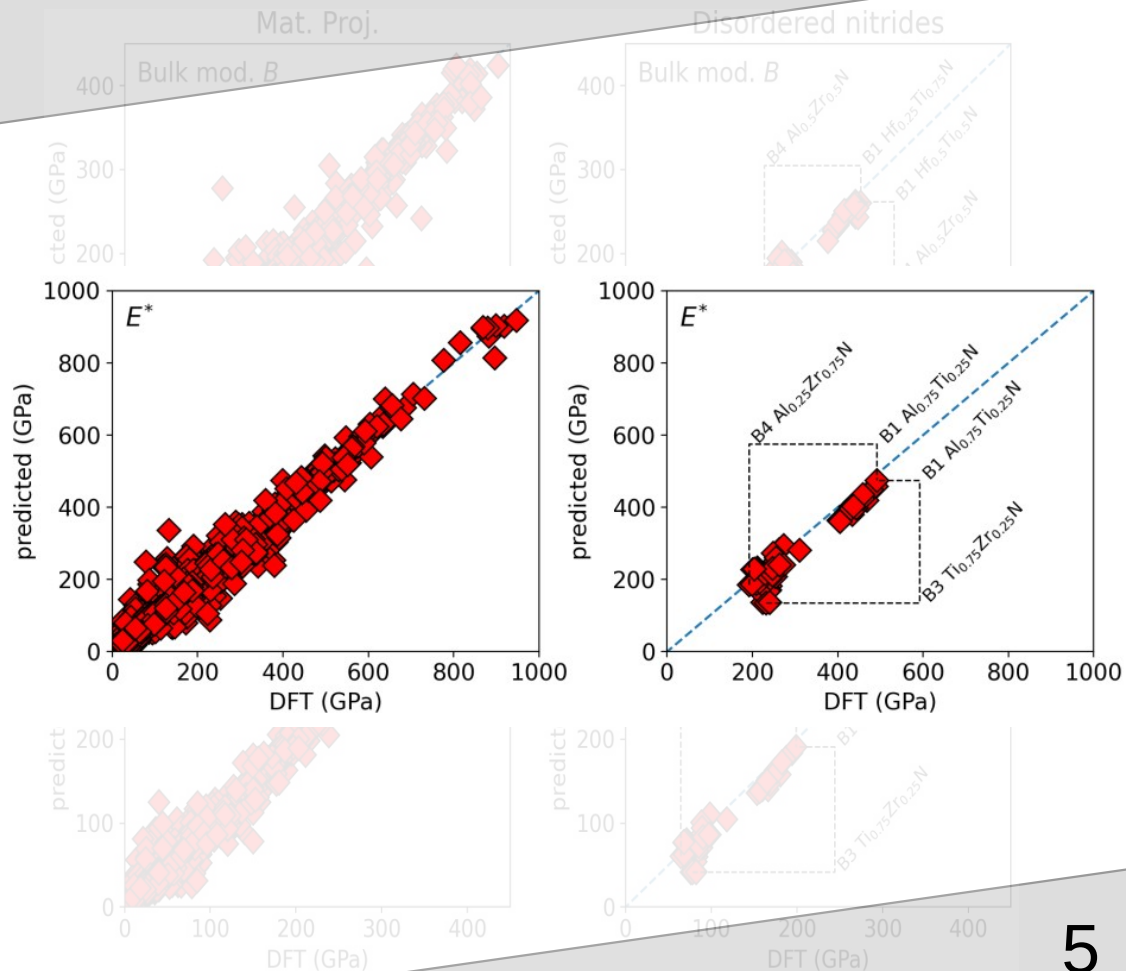
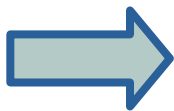
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Thank you for listening!

ferenc.tasnadi@liu.se