Interface induced toughening of nitride superlattices

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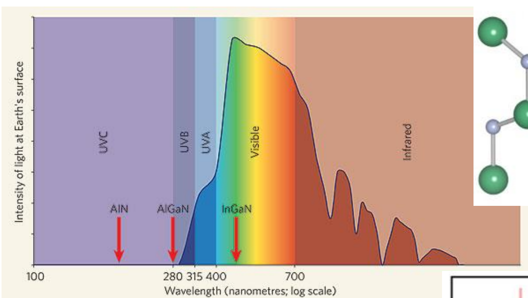
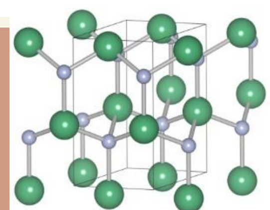
Fascinating nitrides

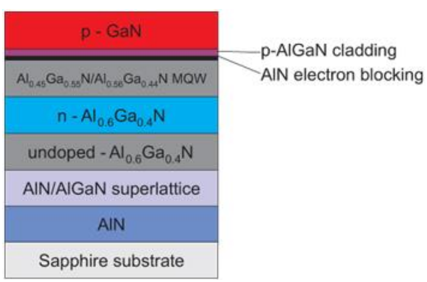
III-V nitrides, e.g. $Al_xGa_{1-x}N$

- semiconductor
- stable alloy in the wurtzite structure
- optoelectronics, sensors

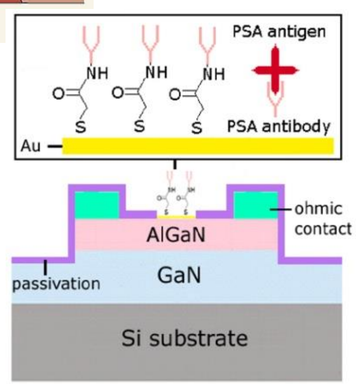




http://www.nature.com/nature/journal/v441/n7091/fig_tab/441299a_F1.html



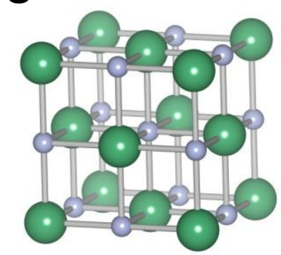
http://www.semiconductor-today.com/news_items/2010/MARCH/NICHIA_310310.htm



http://spie.org/x31865.xml

TM-(Al-)N, e.g. $Ti_xAl_{1-x}N$

- metallic
- unstable when alloyed with Al
- typically cubic (e.g. $Ti_xAl_{1-x}N$ for $x \leq 0.7$, wurtzite for $x \geq 0.7$)
- **protective hard coatings**



http://www.ijs.si/ctp/vrste%20prevlekA.html-12
http://www.sandvik.com

Theory guided materials design

Strategies

Exploring new materials
(alloying, doping, ...)

Tuning the microstructure
(multilayer design, rezidual stress design,...)

Example
hardness of TiN ≈ **34 GPa**

Alloying
TiN + Al (metastable solid solution with 0.66 Al fraction)
hardness of ≈ **37 GPa***

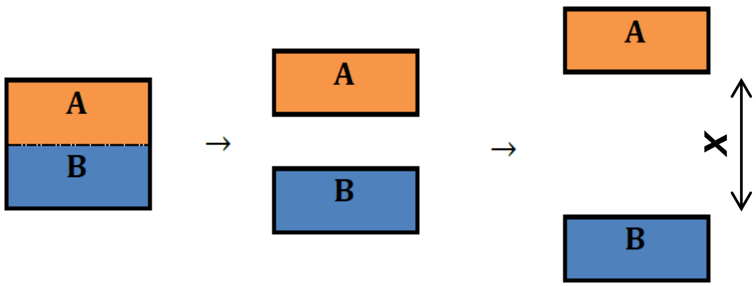
Multilayer design
TiN/VN superlattice:
for bi-layer period 5.2 nm,
hardness of ≈ **55 GPa****

* Mayrhofer et al., Appl. Phys. Lett. 83 (2003) 2049.

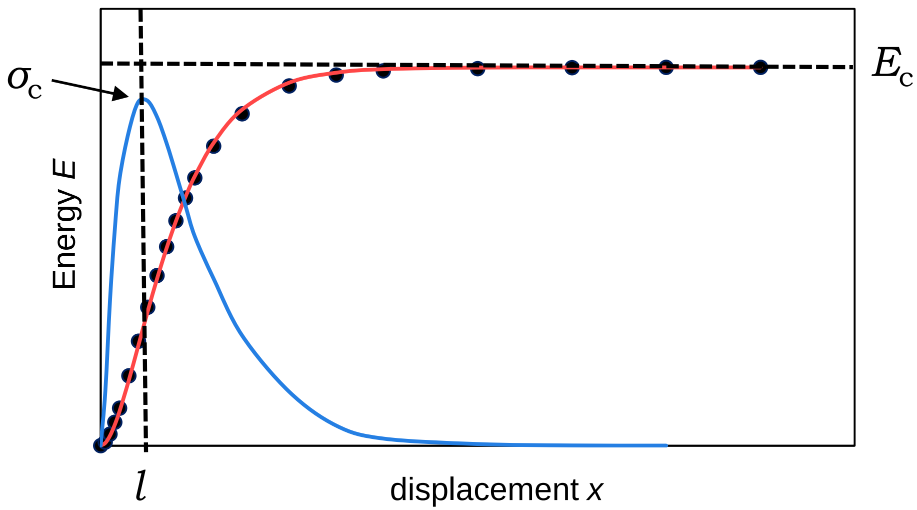
** Helmersson et al., J. Appl. Phys. 62 (1987) 481.

Cleavage energy

Displacement of rigid blocks



Energy *E* computed as a function of the displacement *x*



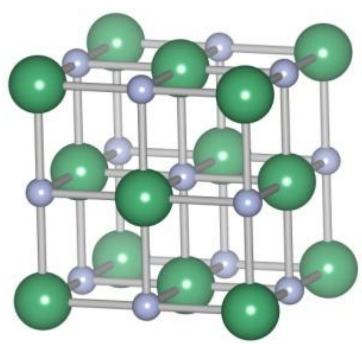
$$E(x) = E_c \left[1 - \left(1 + \frac{x}{l}\right) \exp\left(-\frac{x}{l}\right)\right]$$

$$\sigma(x) = \frac{\mathrm{d}E(x)}{\mathrm{d}x}$$

J.H. Rose, J.R. Smith and J. Ferrante: *Phys. Rev. B*, 28 (4): 1835, 1983.

Cleavage: bulk

		E_c (J/m^2)	l (A)	σ_c (GPa)
bulk	TiN	3.0	0.39	28
	VN	3.2	0.37	32

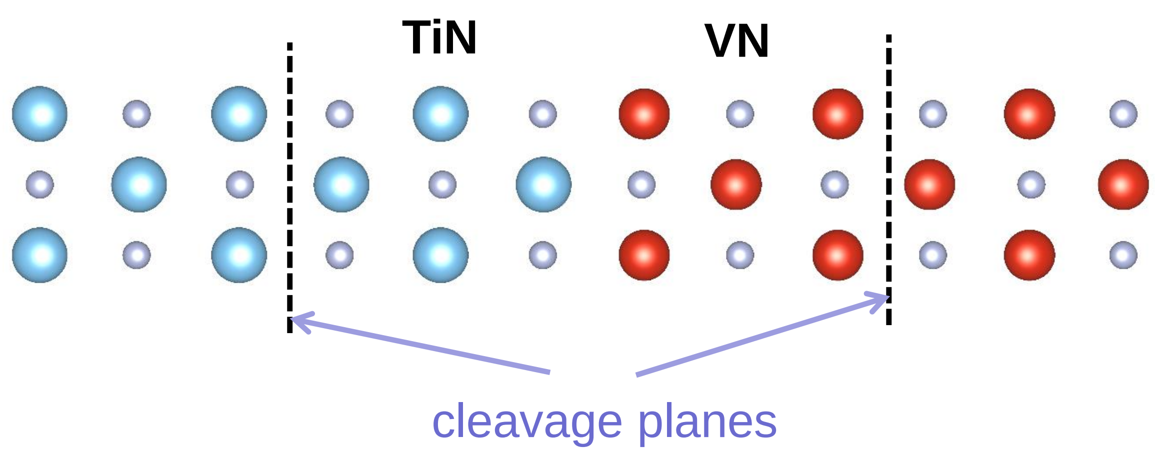


Cleavage: bulk x bilayer

		E_c (J/m²)	l (A)	σ_c (GPa)
bulk	TiN	3.0	0.39	28
	VN	3.2	0.37	32
bilayer	TiN	2.9	0.37	29
	VN	4.0	0.35	41

interface induced toughening?

bilayer with (100) interface



P. Řehák, M. Černý and D. Holec : Surf. Coat. Technol., 325: 410, 2017.

Cleavage: bulk x bilayer

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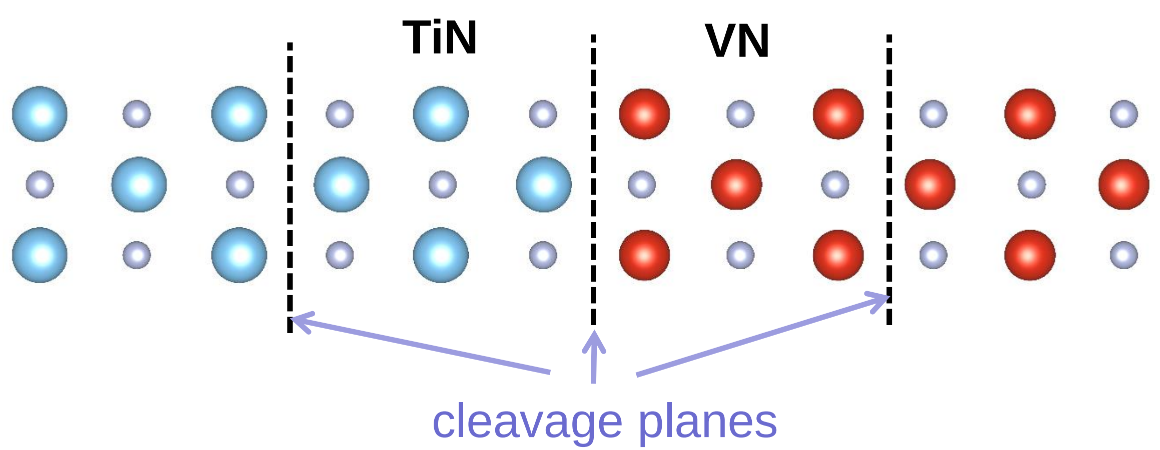
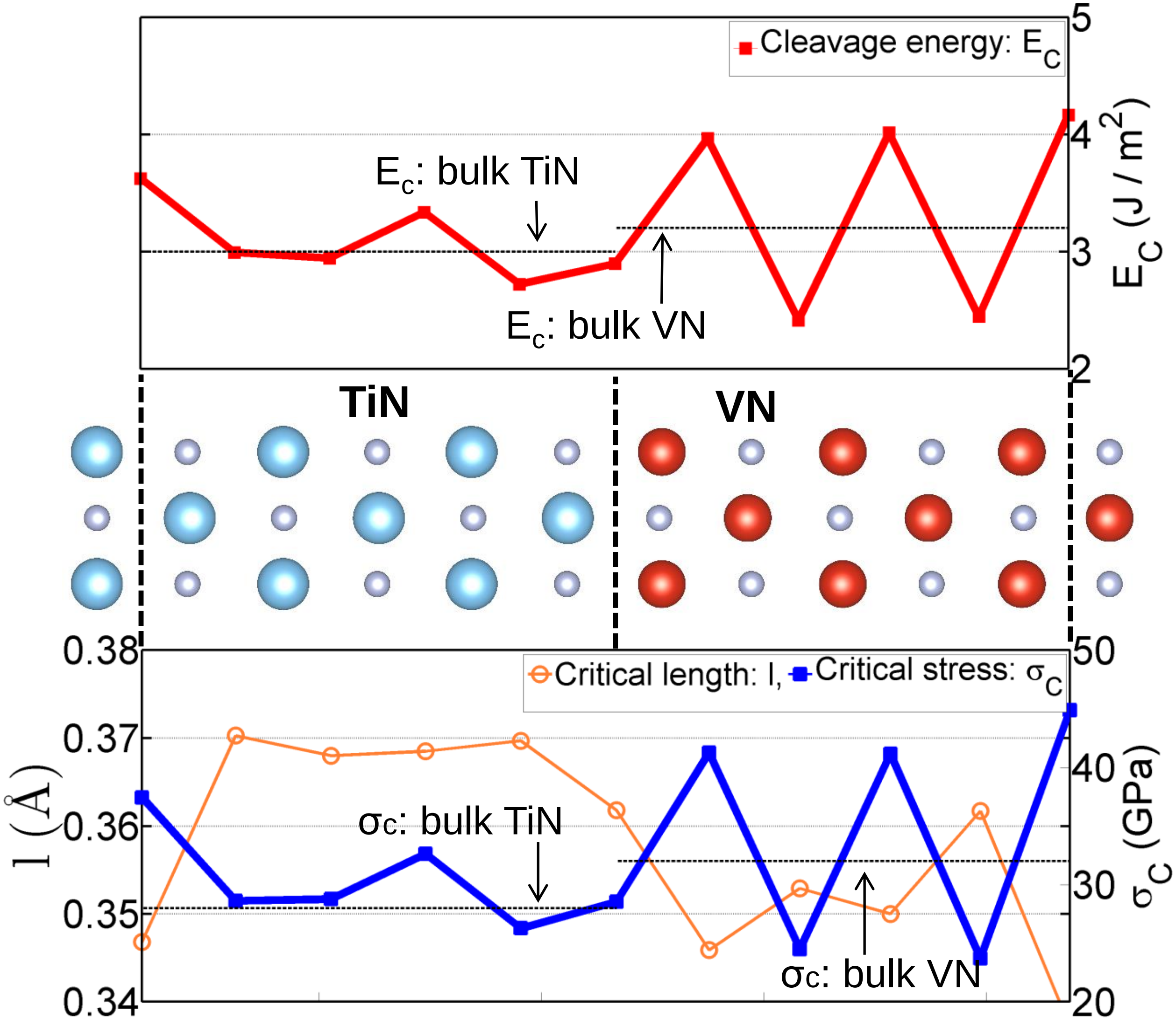
	VN	3.2	0.37	32
bilayer	TiN	2.9	0.37	29
	VN	4.0	0.35	41
	interface	**2.9**	**0.36**	**29**

interface induced toughening?

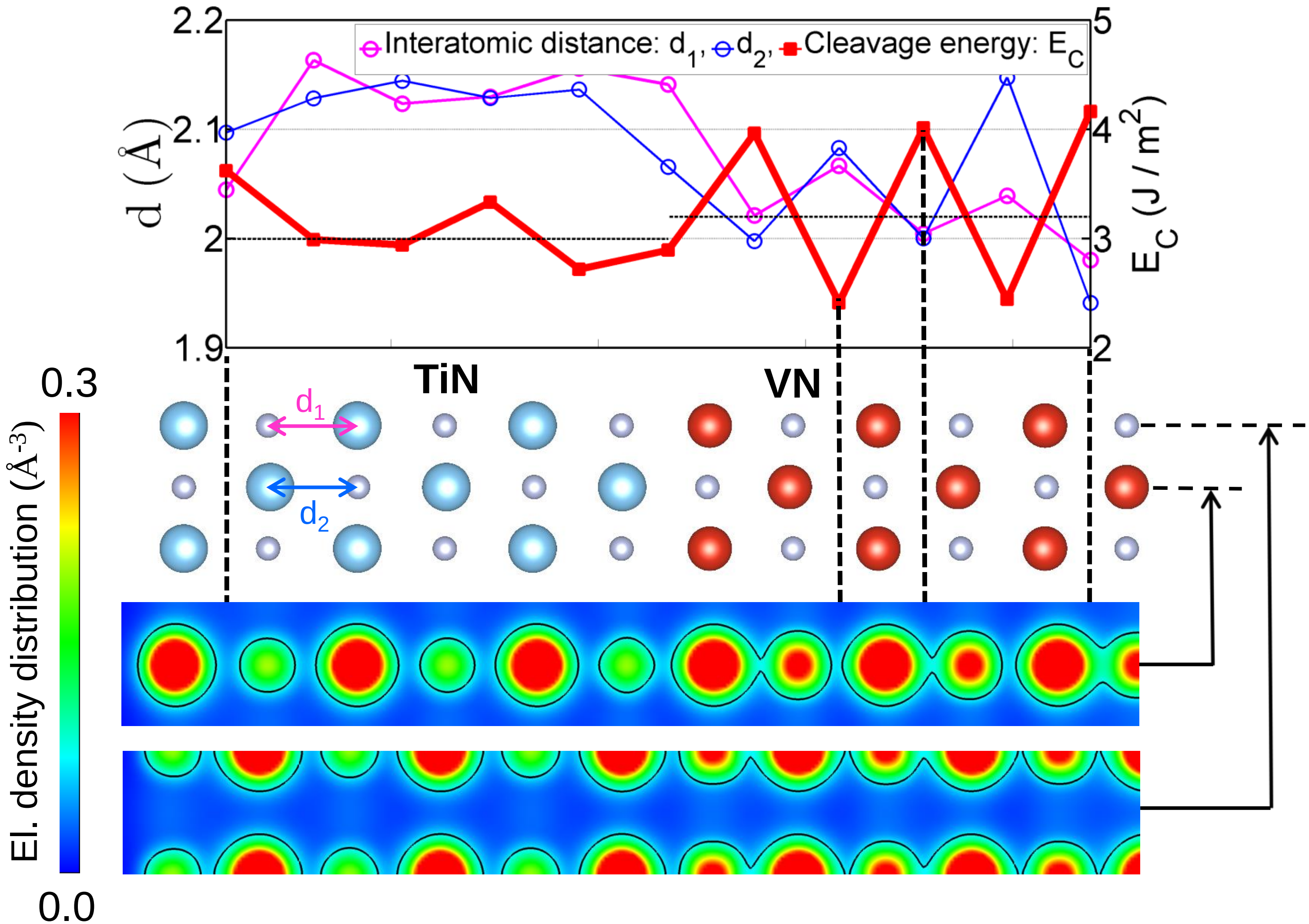


P. Řehák, M. Černý and D. Holec : Surf. Coat. Technol., 325: 410, 2017.

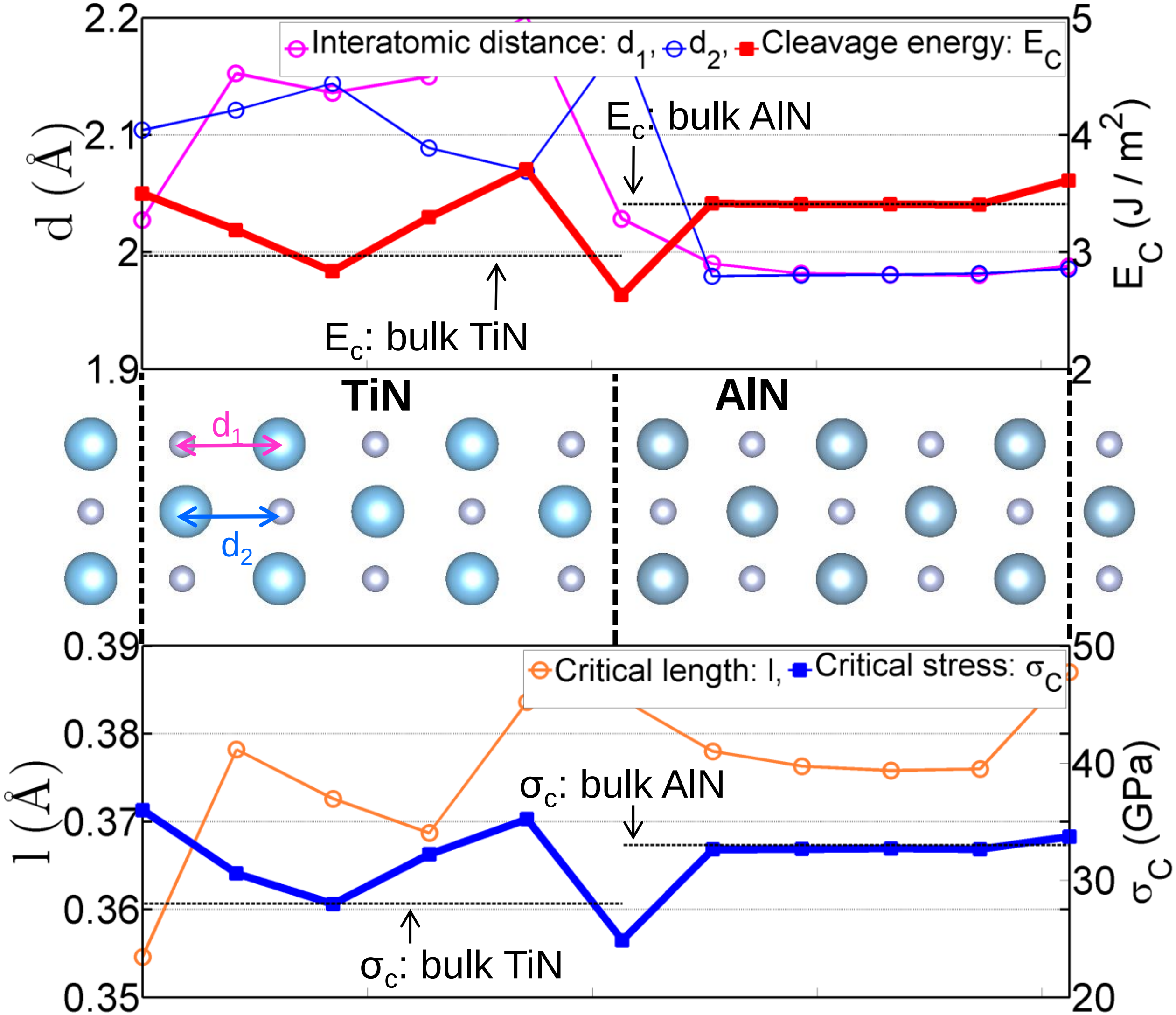
Cleavage of TiN / VN (100) bilayer



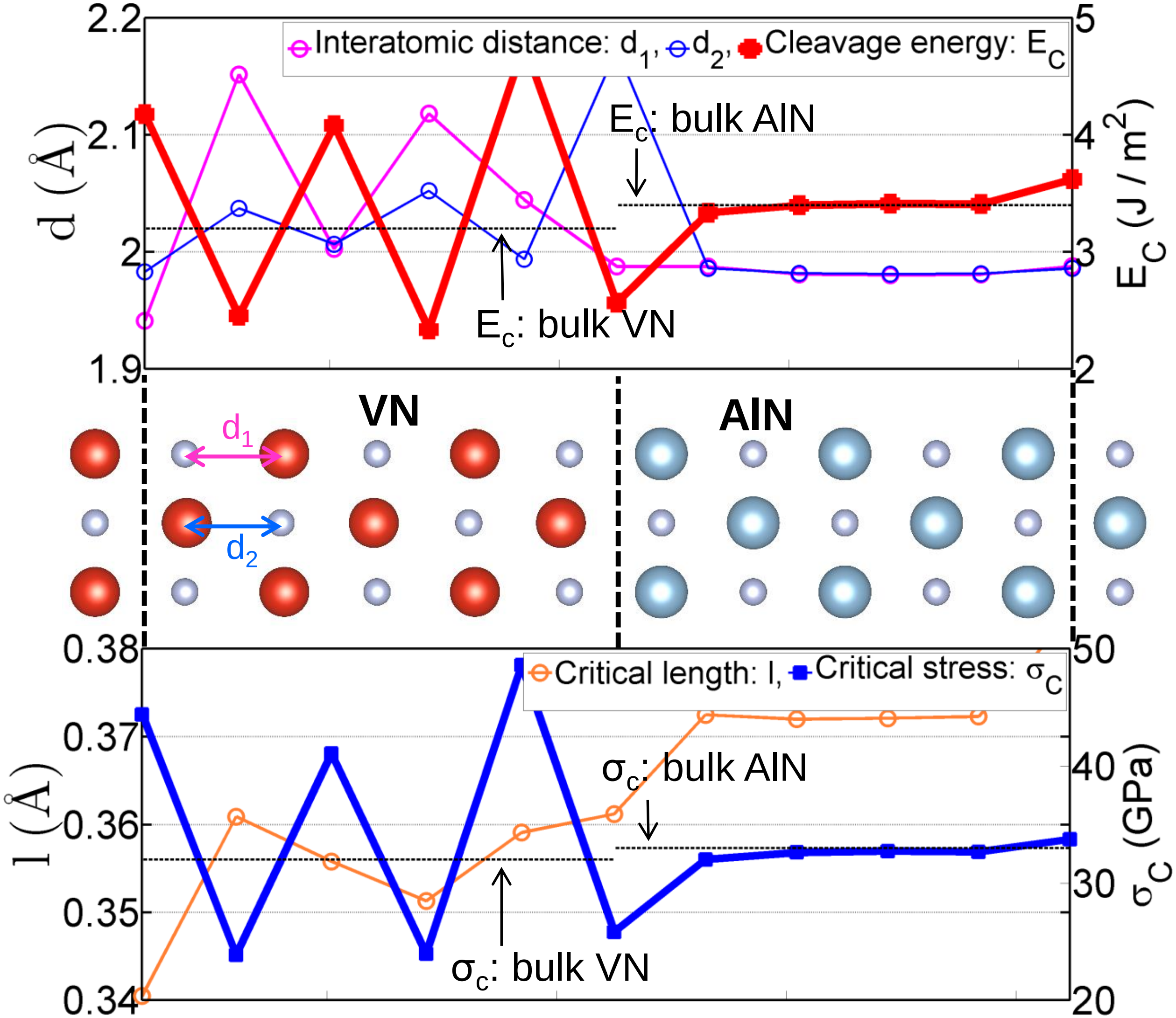
Cleavage of TiN / VN (100) bilayer



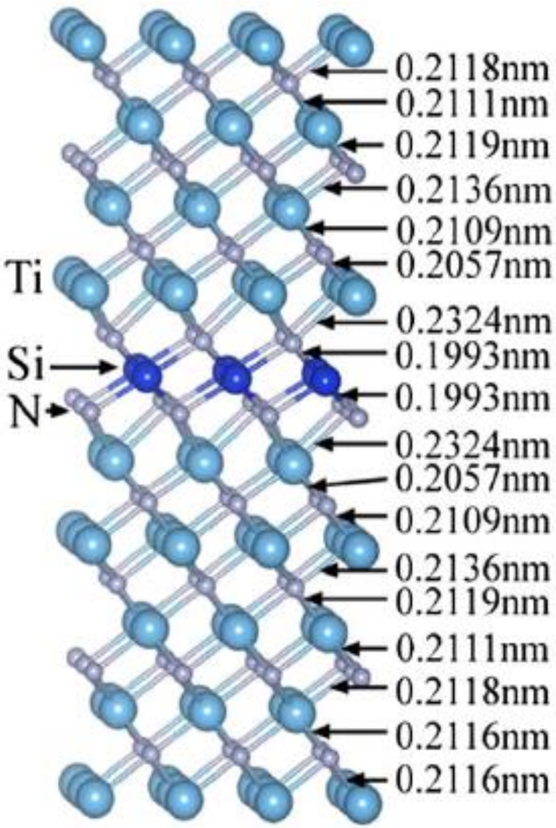
Cleavage of TiN / AlN (100) bilayer

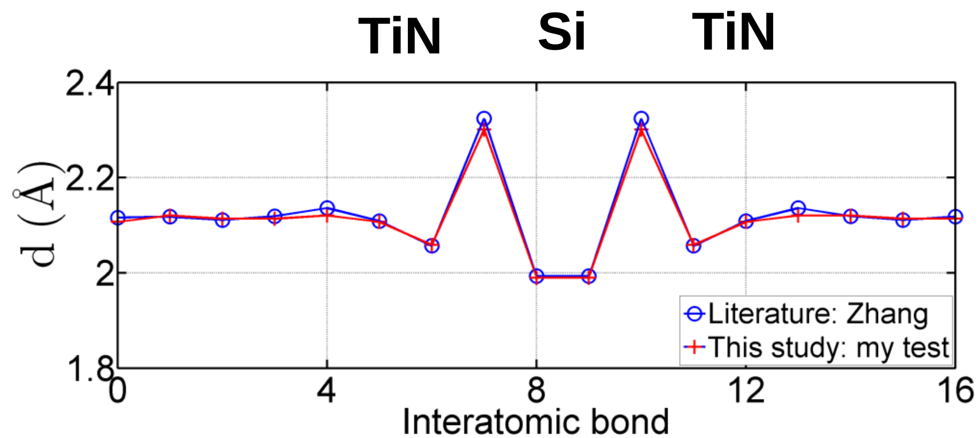


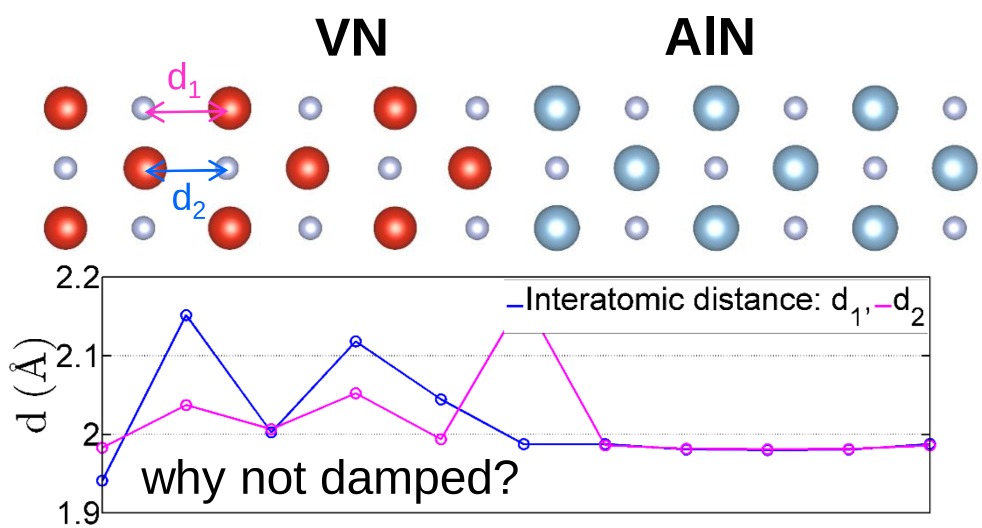
Cleavage of VN / AlN (100) bilayer



Friedel oscillations: literature vs. present study

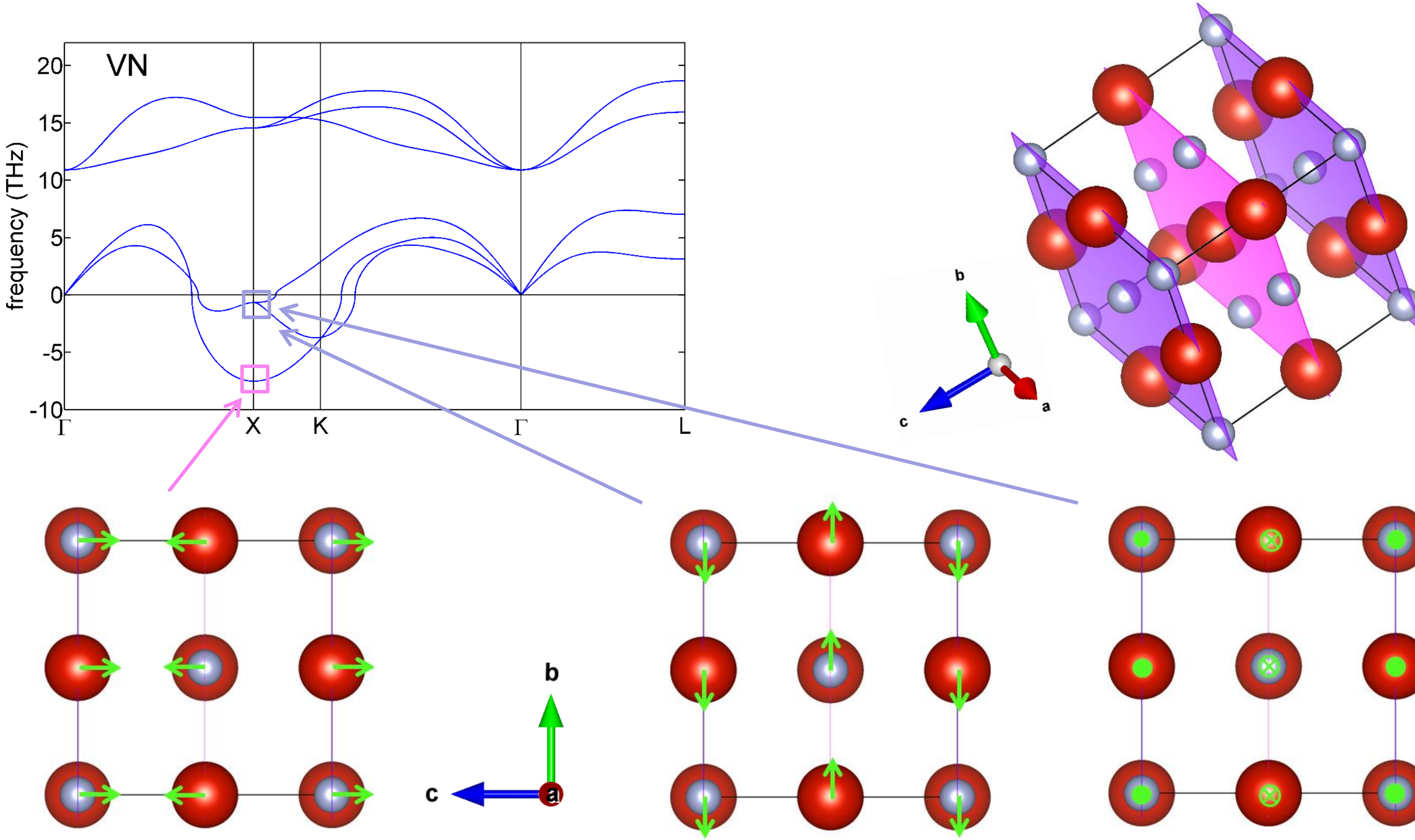






R. F. Zhang, A. S. Argon and S. Veprek: *Phys. Rev. Lett.*, 102: 015503, 2009.

Driving “force” of oscillations: bulk VN



Conclusions

Cleavage properties of AlN, VN, TiN layers were studied from first principles.

• Interplanar distance (perpendicular to the interface) changes from plane to plane in VN and TiN where VN is very prone to the oscillations of distances.

• Cleavage energy and critical stress are strongly anticorrelated with interplanar distance

• Huge oscillations (without any damping) in VN layer are allowed by the microscopic instability of cubic VN.

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