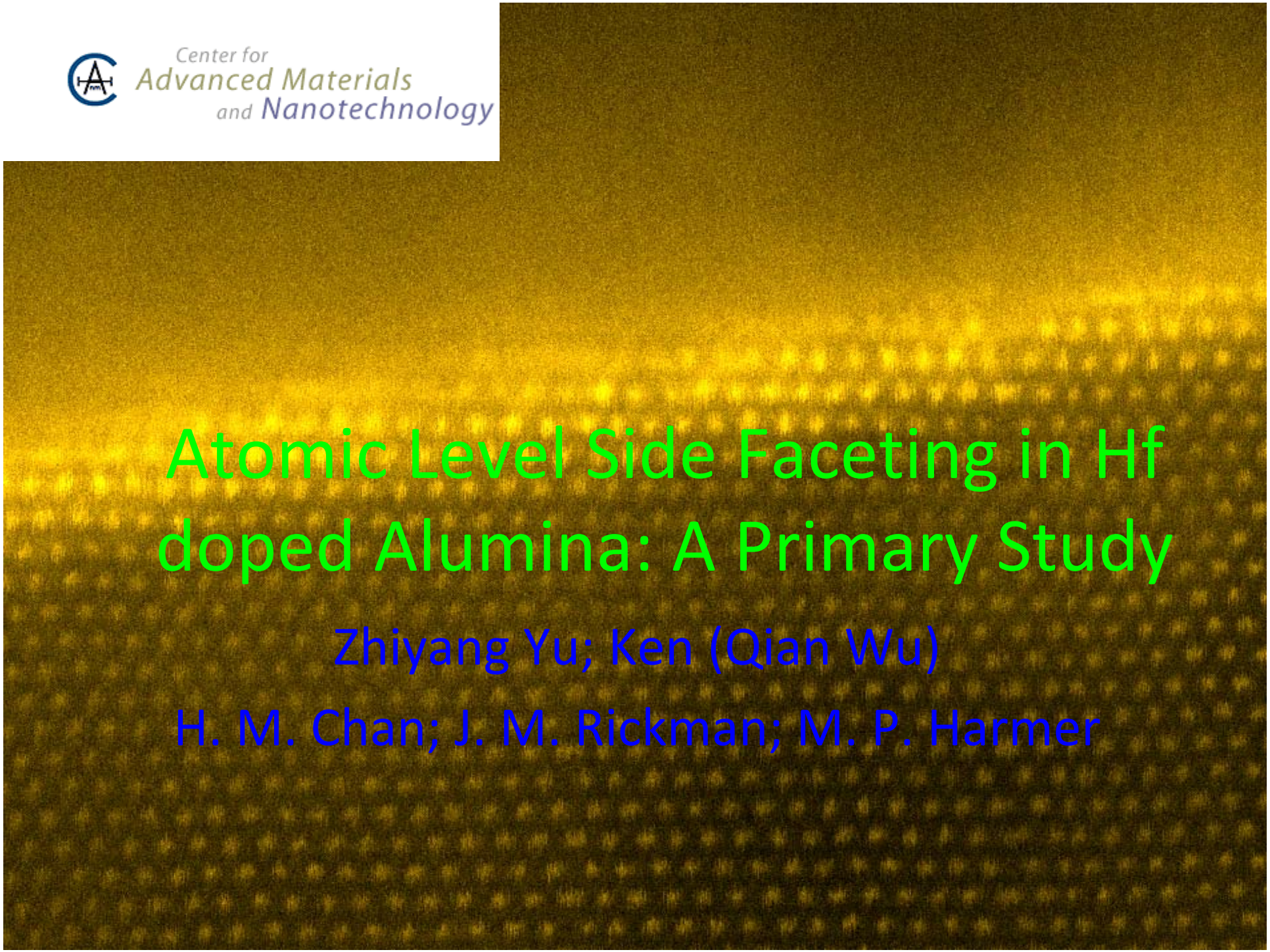
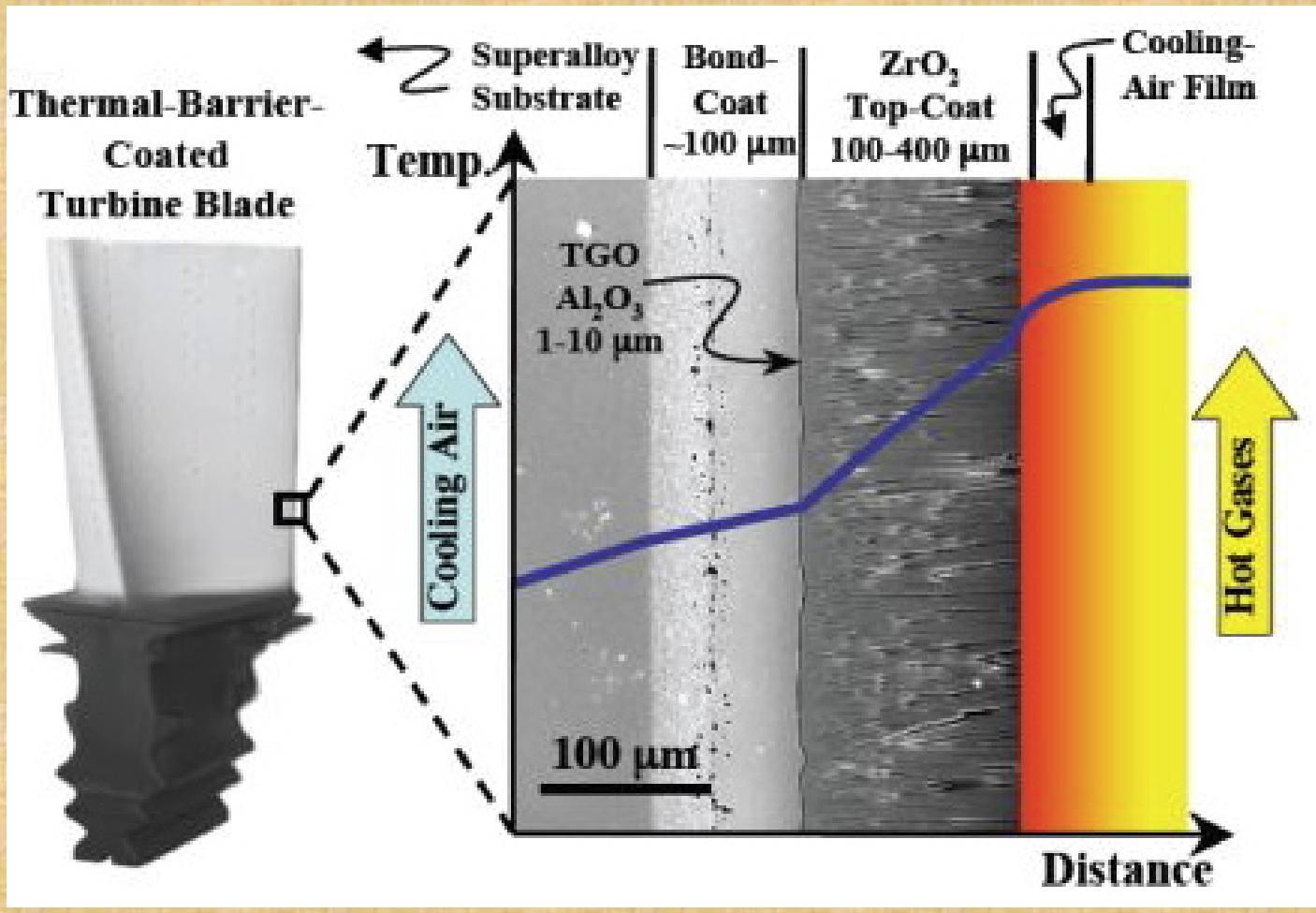

Center for
Advanced Materials
and Nanotechnology
Atomic Level Side Faceting in Hf doped Alumina: A Primary Study
Zhiyang Yu; Ken (Qian Wu)
H. M. Chan; J. M. Rickman; M. P. Harmer

Outline

- Introduction
- General observation of Hf-doped GB
- Atomic scale side faceting in the GB
- Conclusions

Turbine blades and TBCs



Thermal barrier coatings (TBCs) for gas-turbine engine applications

Padture *et al.*, Science, vol 296, 2002

With RE additions…

Reactive element additives (e.g. Y,Hf) are beneficial to oxidation behavior of alumina formers.

- **Improving adhesion of scale**
- **Slowing transport kinetics**
- **Modifying microstructure of scale**

Outline

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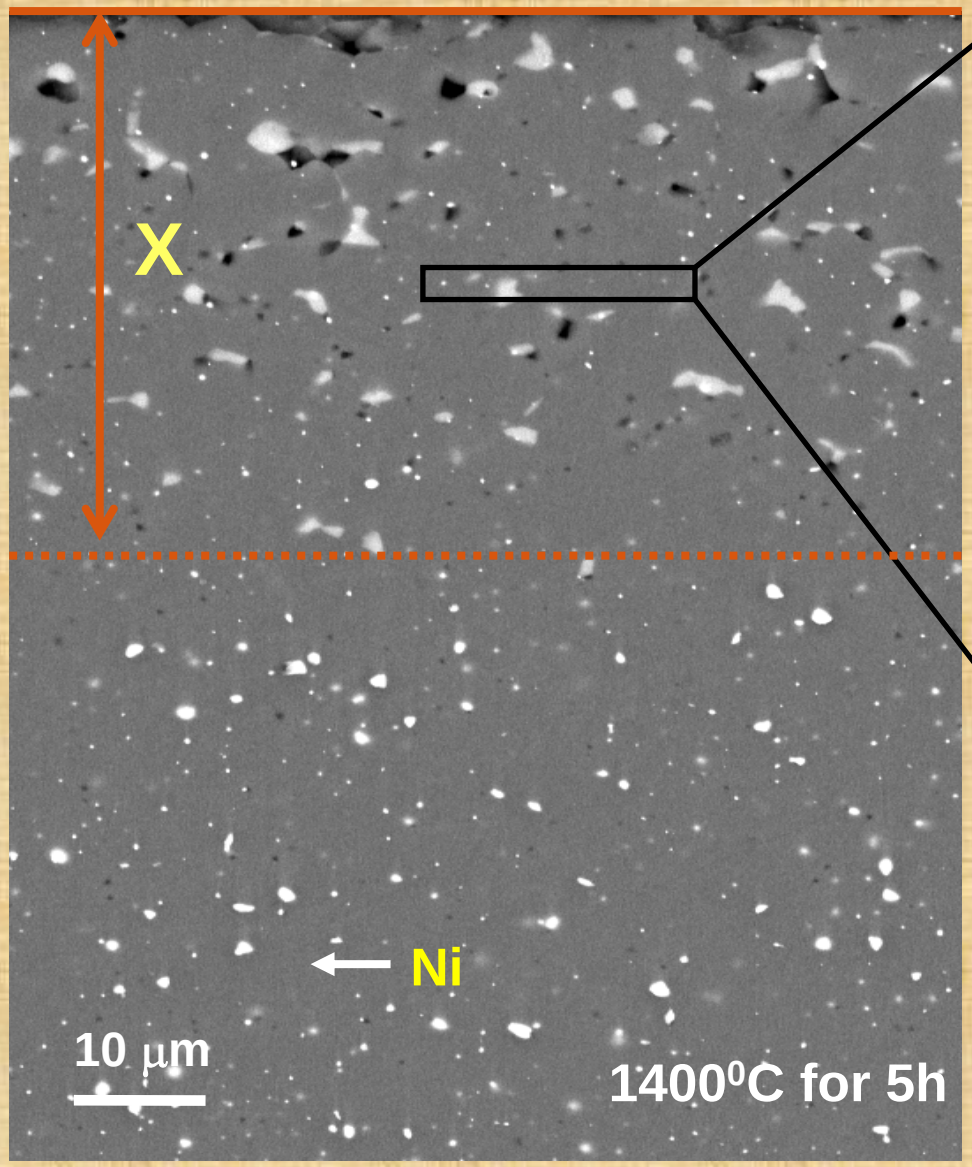
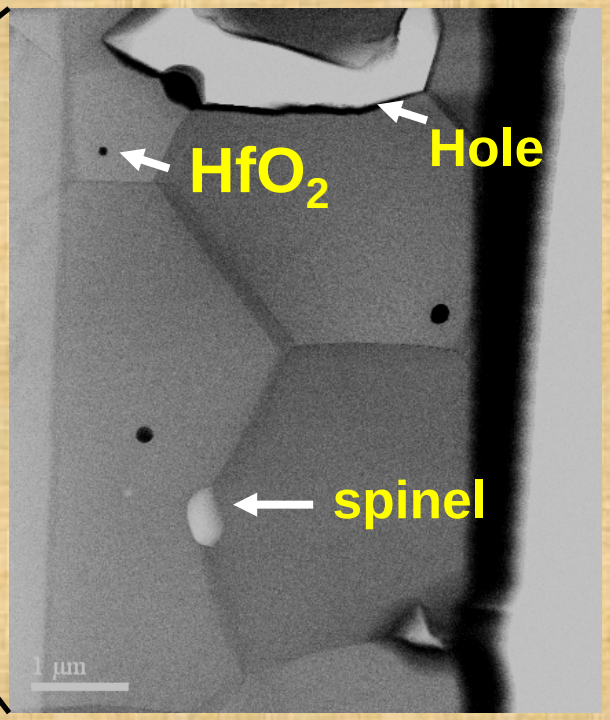
- General observation of Hf-doped GB
- Atomic scale side faceting in the GB
- Conclusions

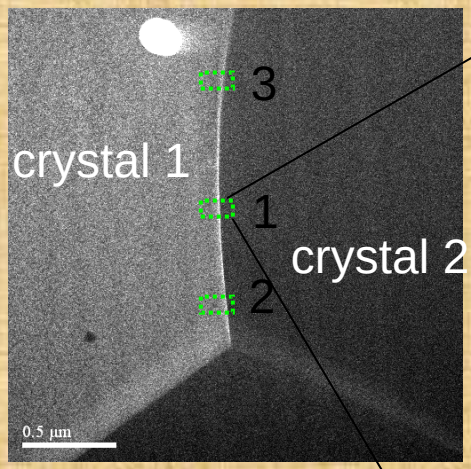
FIB Sample – 500ppm Hf doped

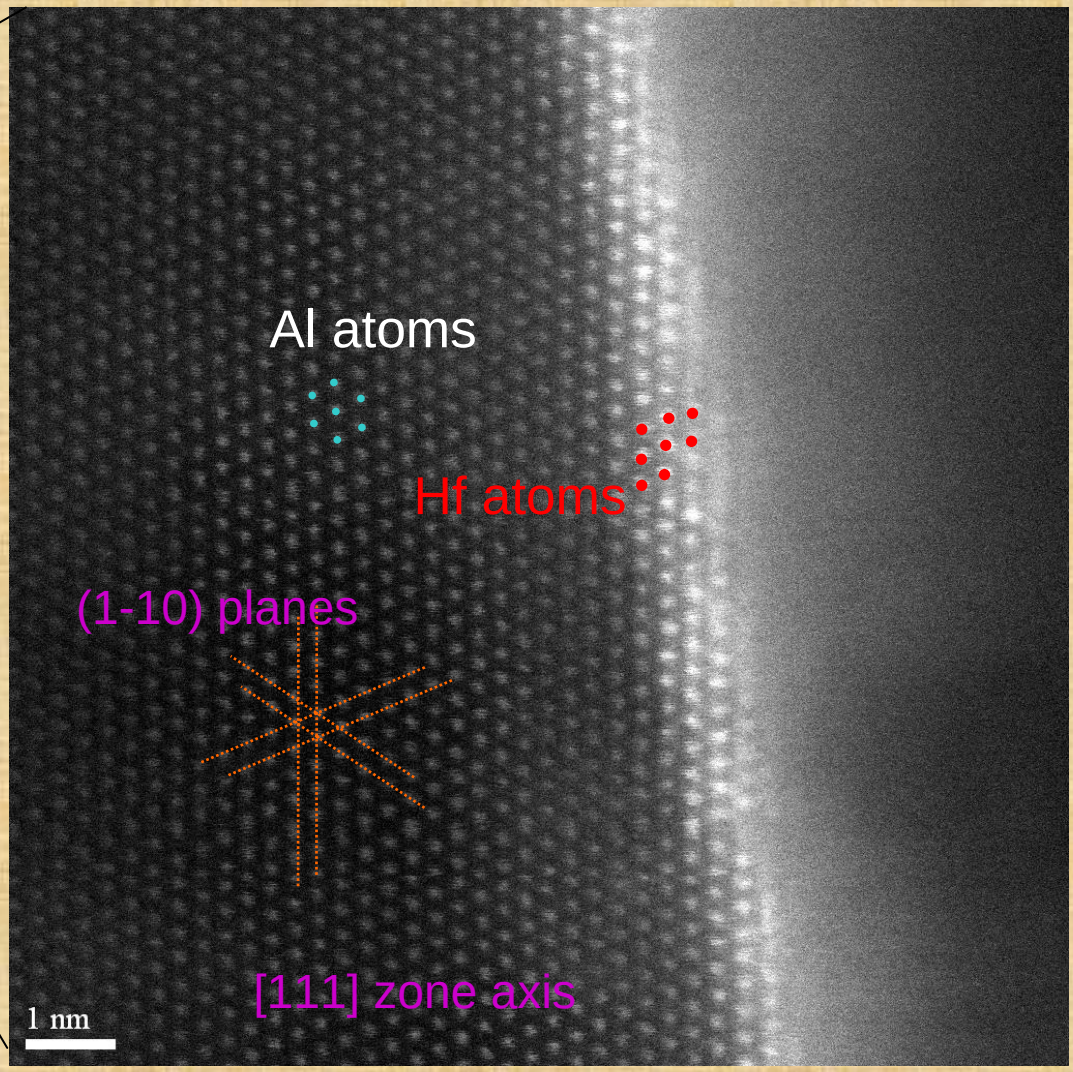




- 500ppm Hf-0.5vol% Ni – Al_2O_3
- 1400^0C for 5h
- Inside the Oxidation Region

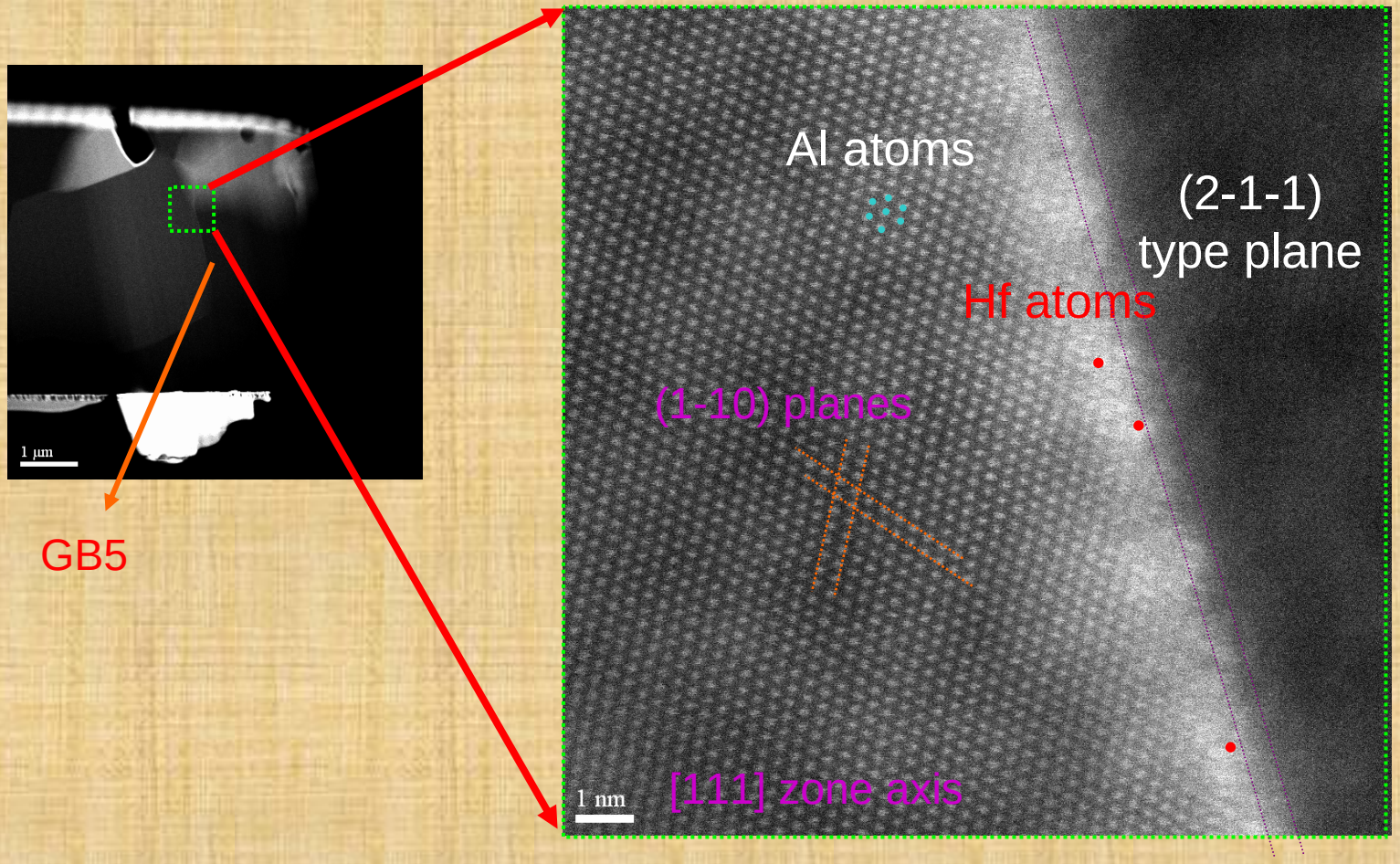
4 GBs Observed with Surface Steps





- **Hf substitutes Al atoms**
- **Atomic Side Faceting**

1 Rough Low Energy Surface GB observed

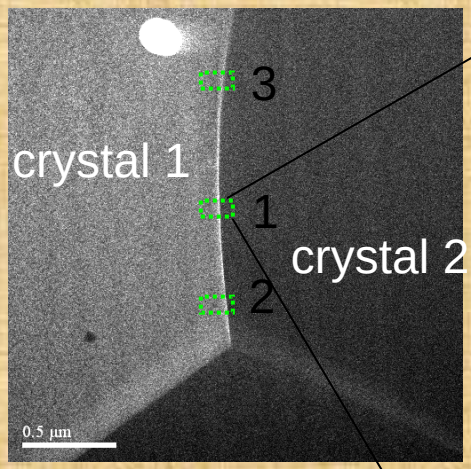


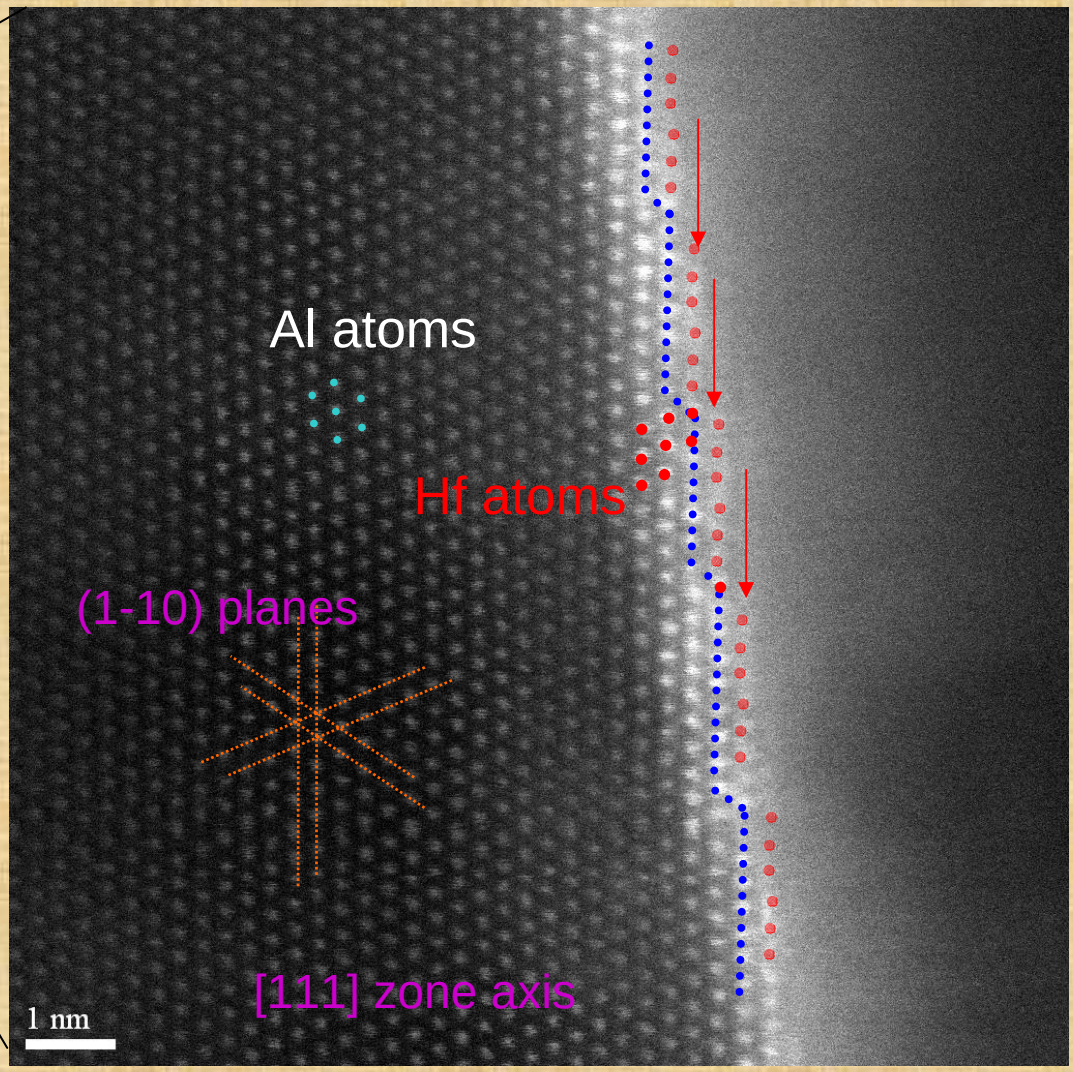
- **No steps**
- **No obvious ordered segregation**

Outline

- Introduction
- General observation of Hf-doped GB
- Atomic scale side faceting in the GB
- Conclusions

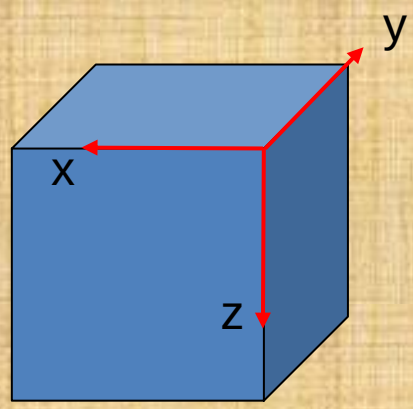
Ordered Hf segregation





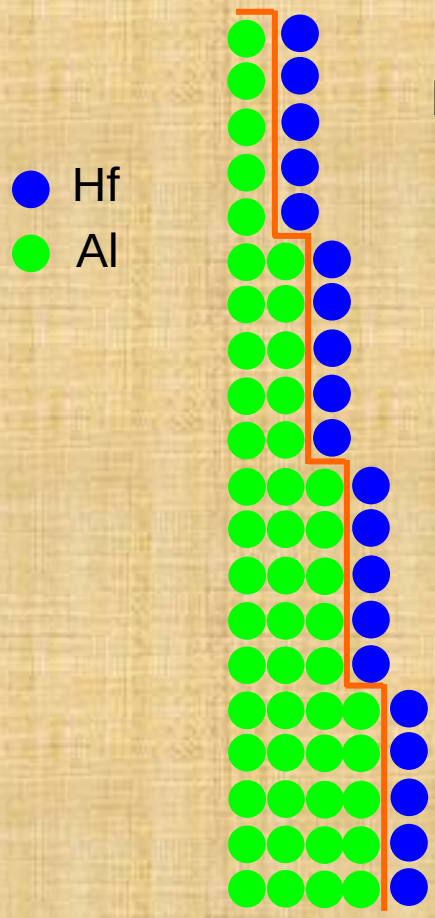
■ **one atomic height steps in the beam direction**

Models of steps-model1



steps in z direction
(z: beam direction)

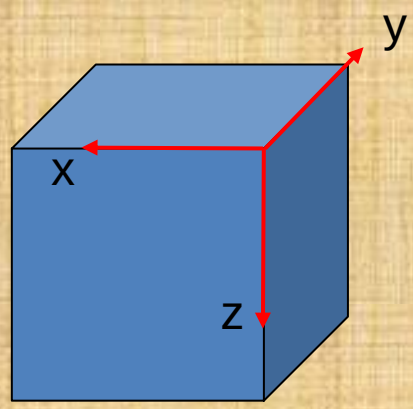
Model1



beam direction

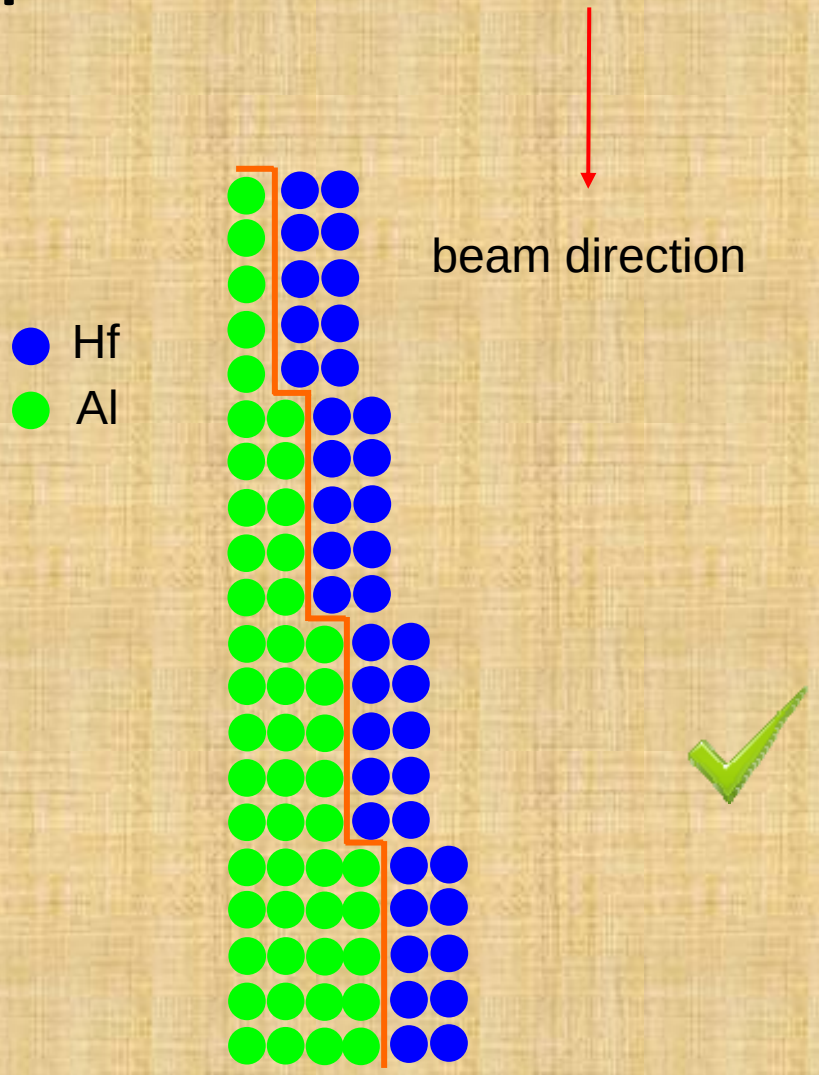
one atom scale step; one layer

Models of steps—model2



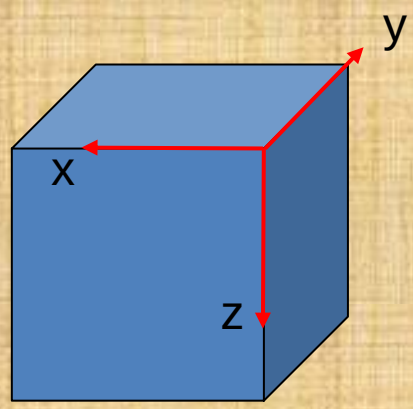
steps in z direction
(z: beam direction)

Model2



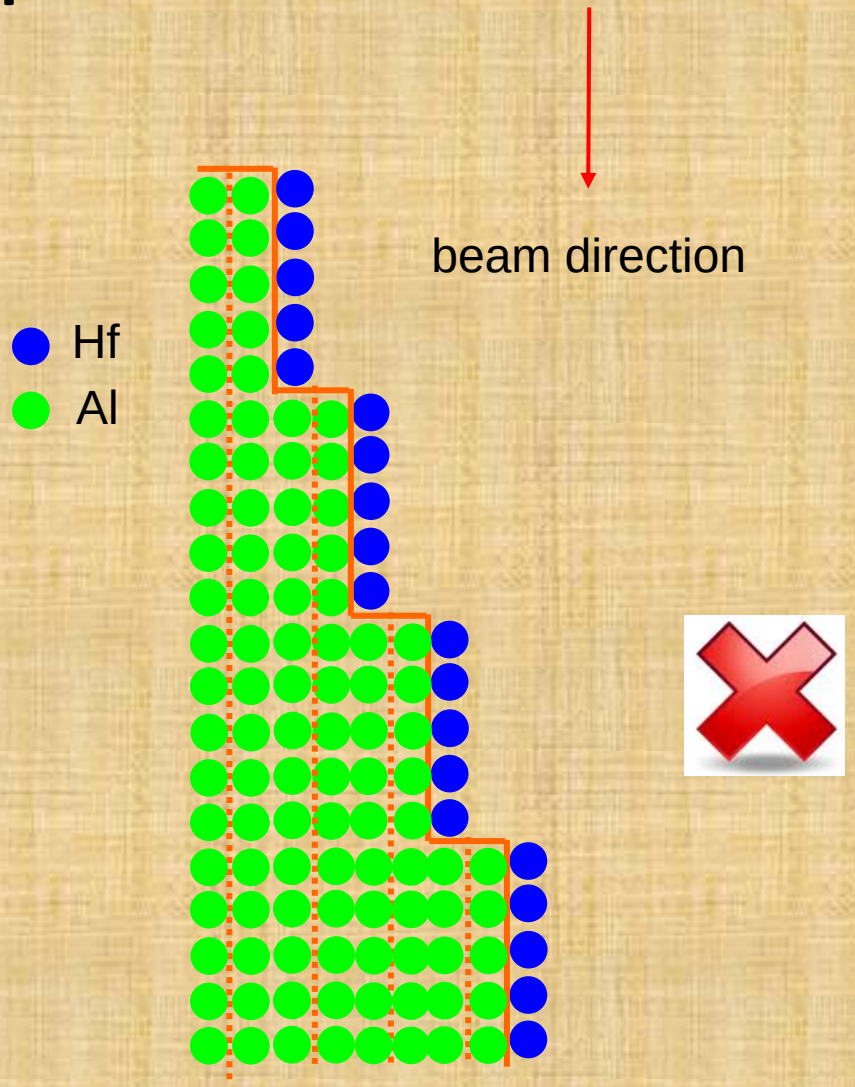
one atom scale step; double layer

Models of steps—model3



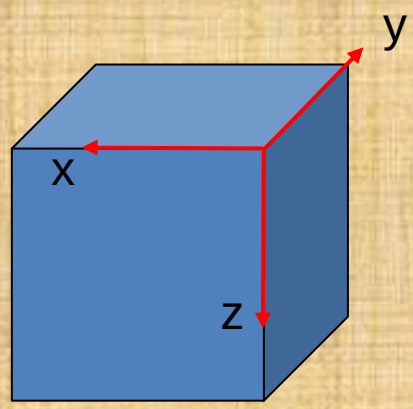
steps in z direction
(z: beam direction)

Model3

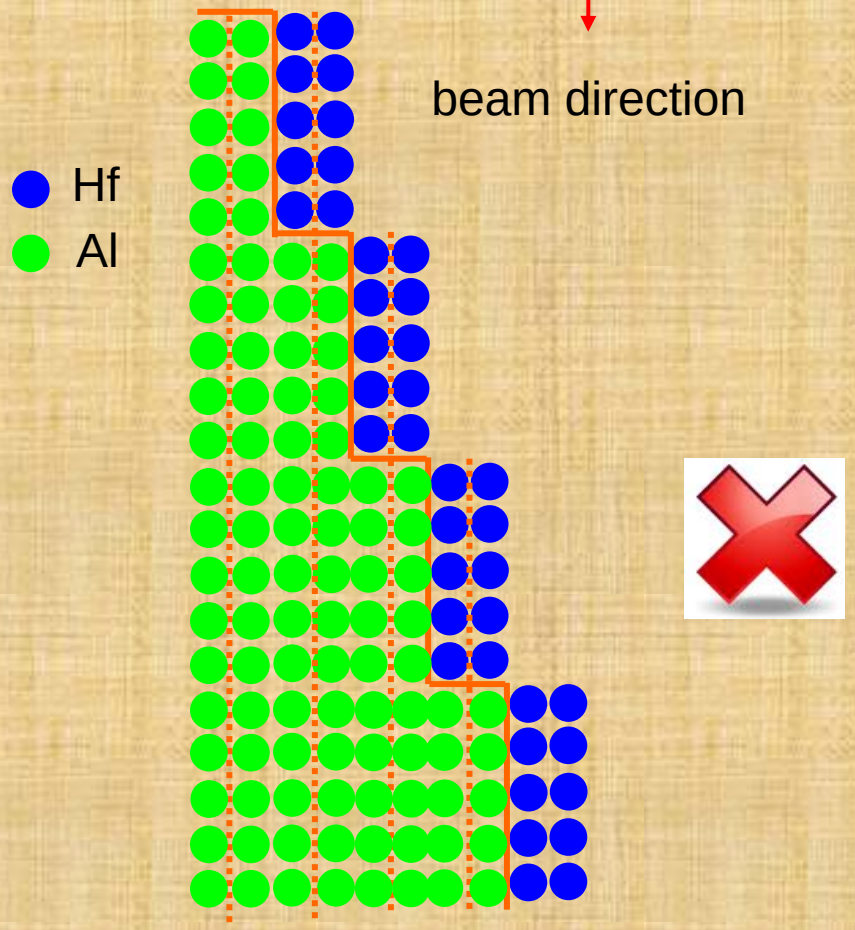


twp atom scale step; double layer

Models of steps—model4



steps in z direction
(z: beam direction)



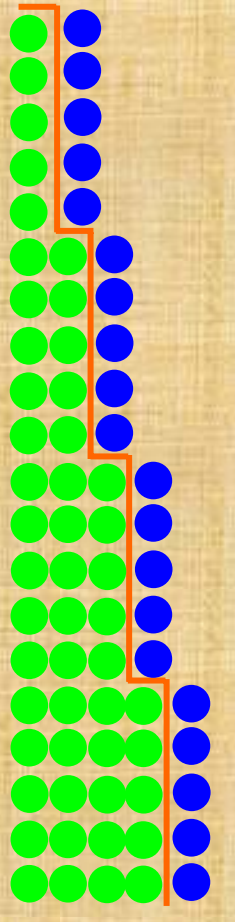
twp atom scale steps; double layer

Model4

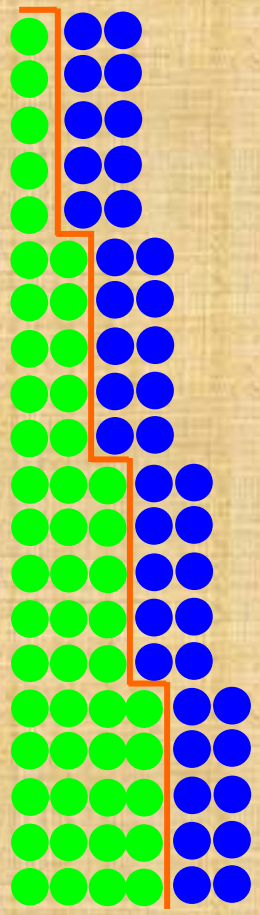
Model1 Vs Model2

beam direction

Hf
Al



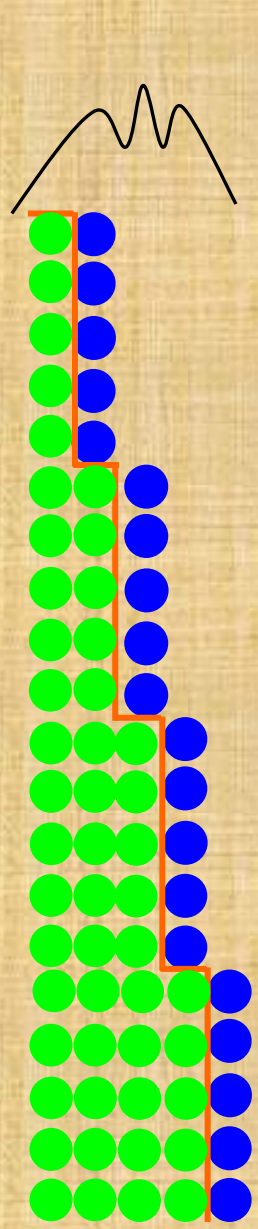
Model1
one atom scale step; one layer segregation



Hf
Al

Model2
one atom scale step; double layer segregation

Model1 VS Model2

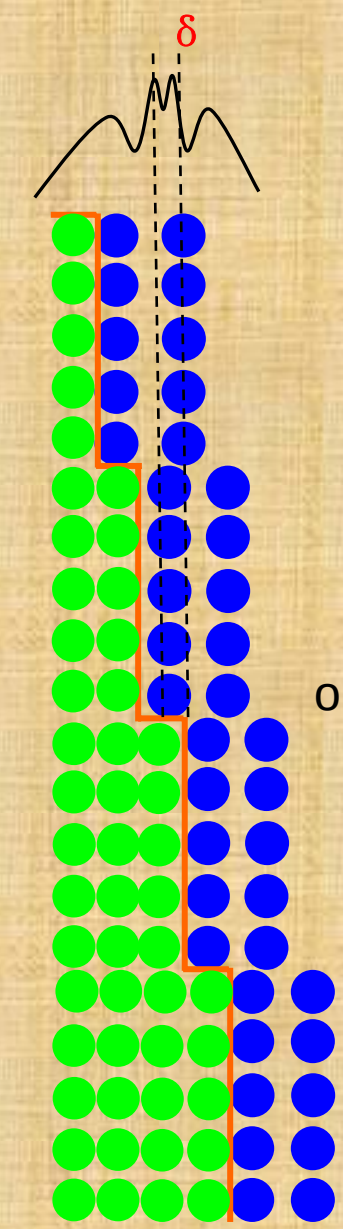


beam direction

Model1

one atom scale step

monolayer



Model2

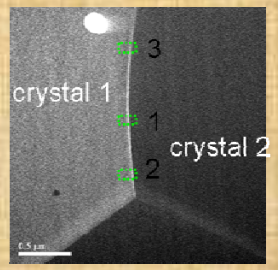
one atom scale step

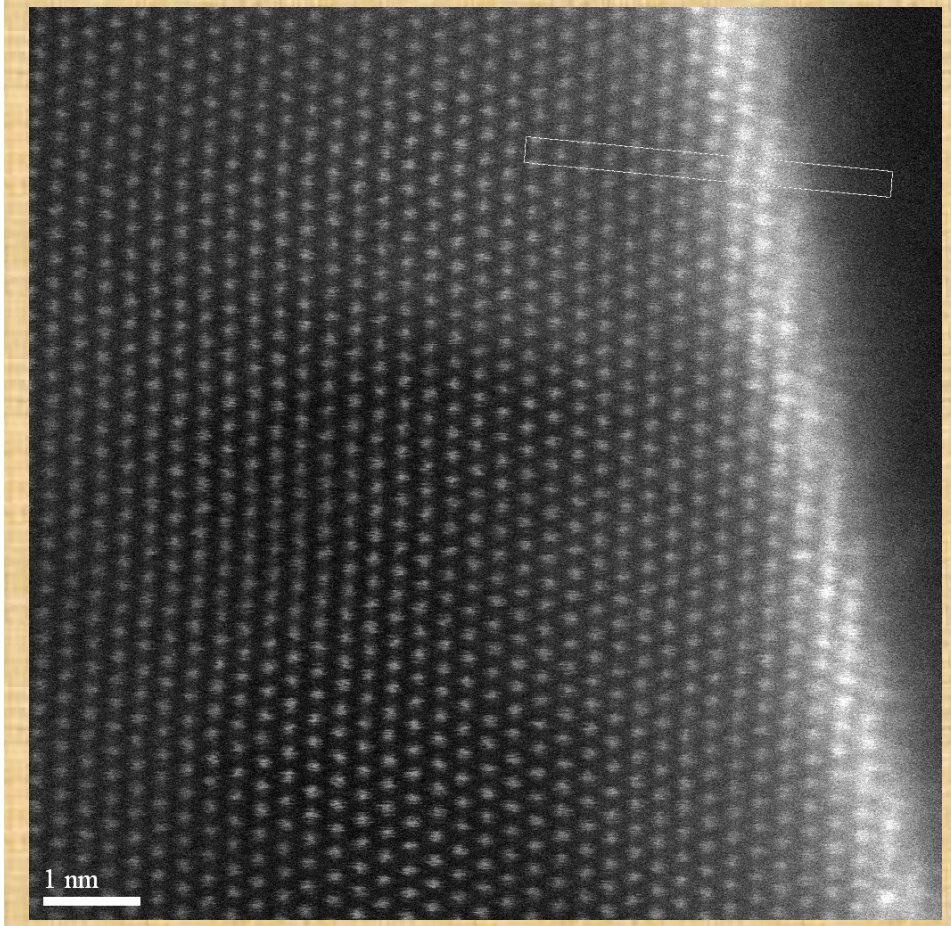
double layer

Hf

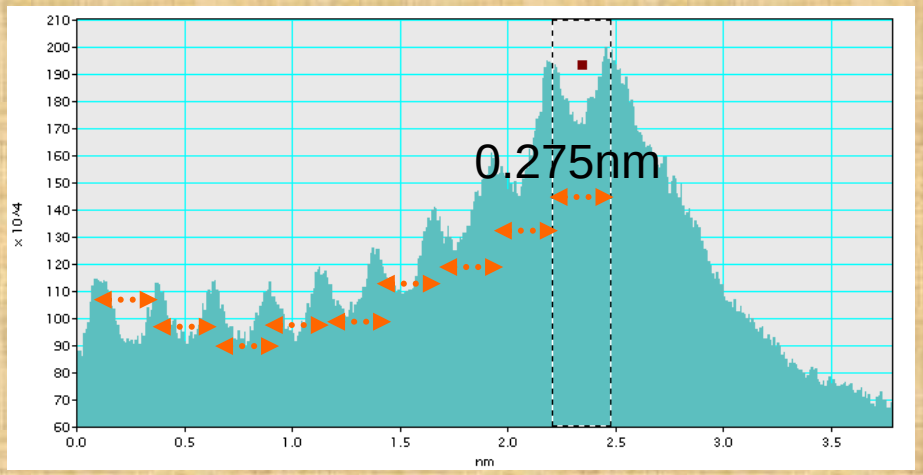
Al

Model1 VS Model2





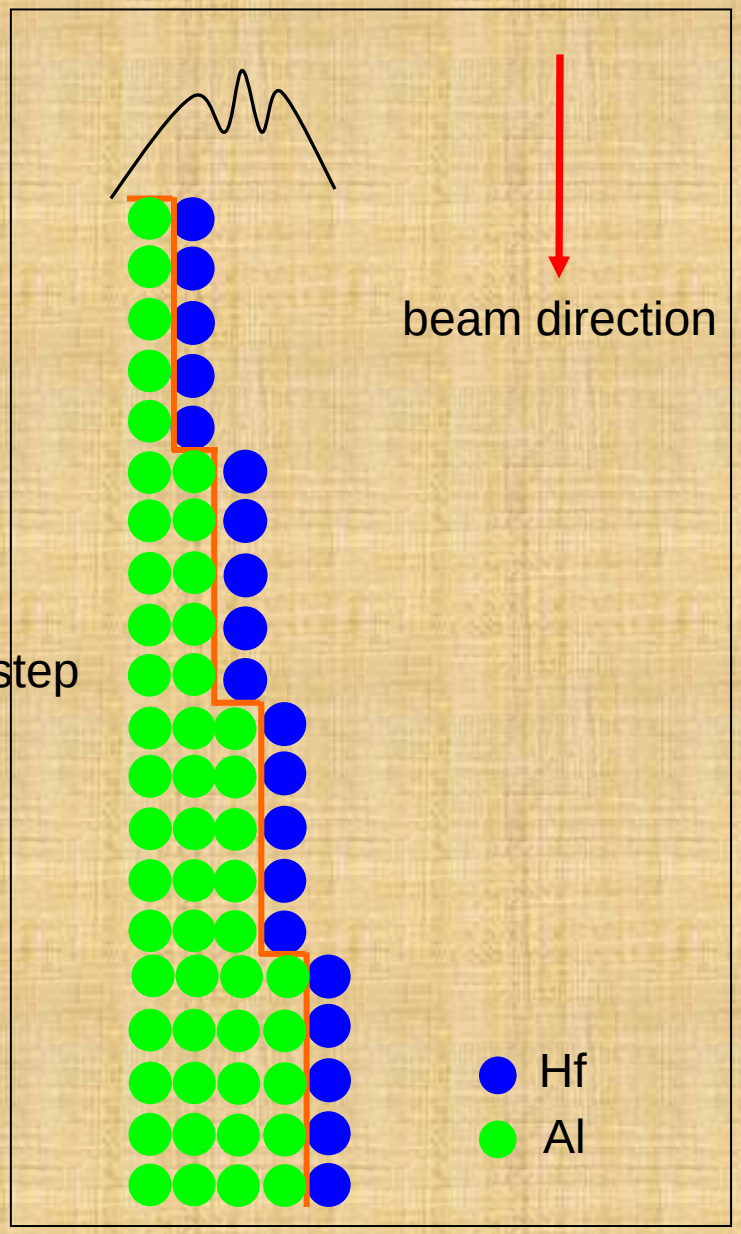
High resolution HAADF image of Hf doped sample



line profile

■**No peak shift or split observed**

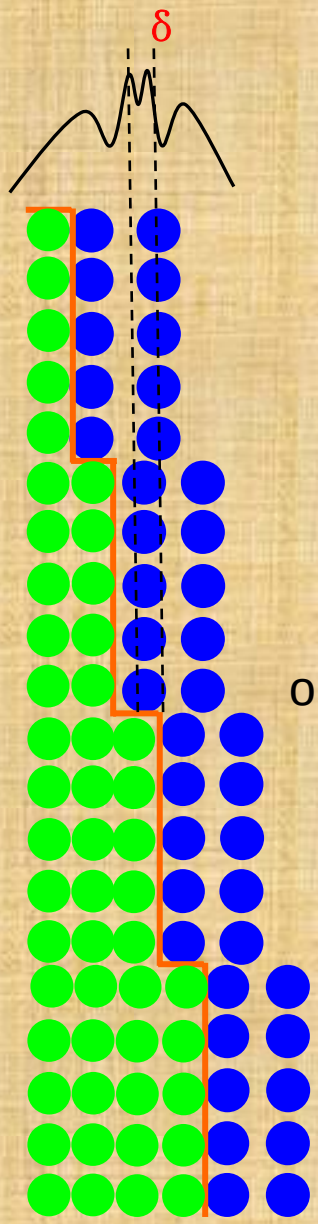
Two Possible Models of Steps



model1

one atom scale step

monolayer

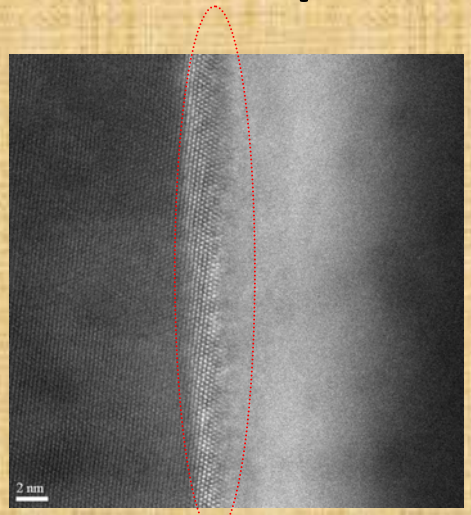


model2

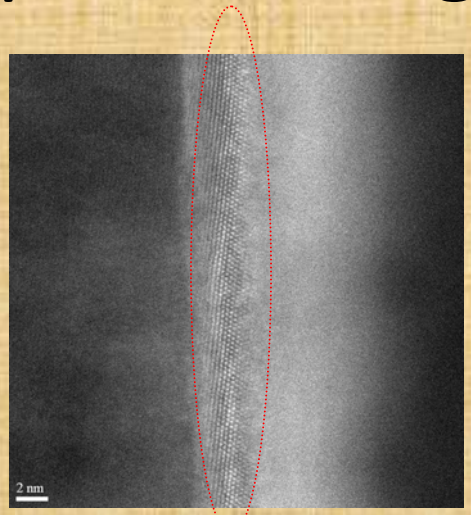
one atom scale step

double layer

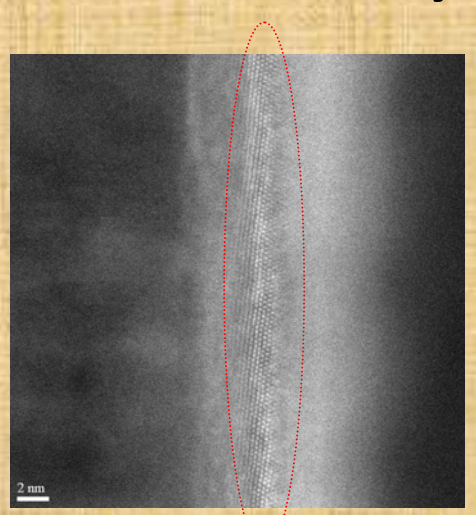
Sharp steps-A through focus study



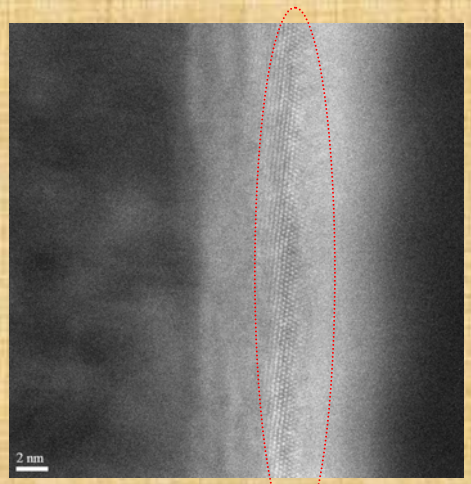
-20nm



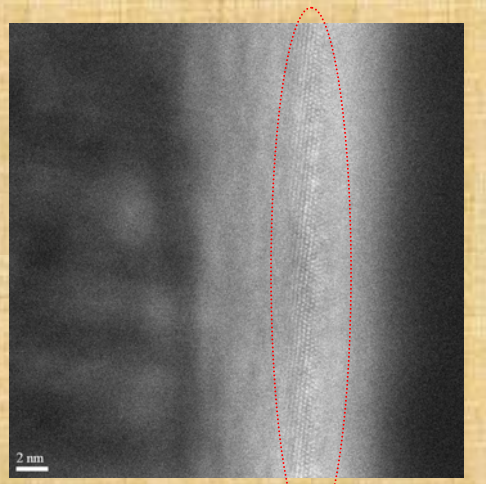
-60nm



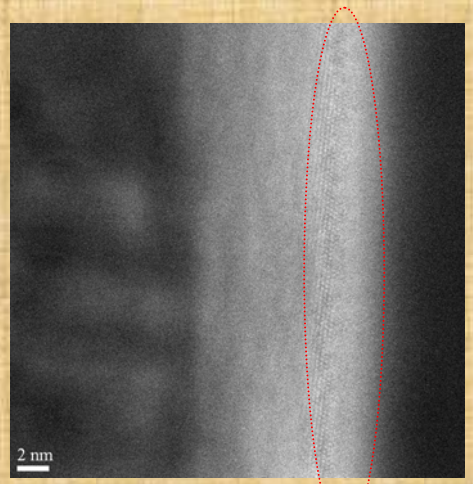
-100nm



-140nm



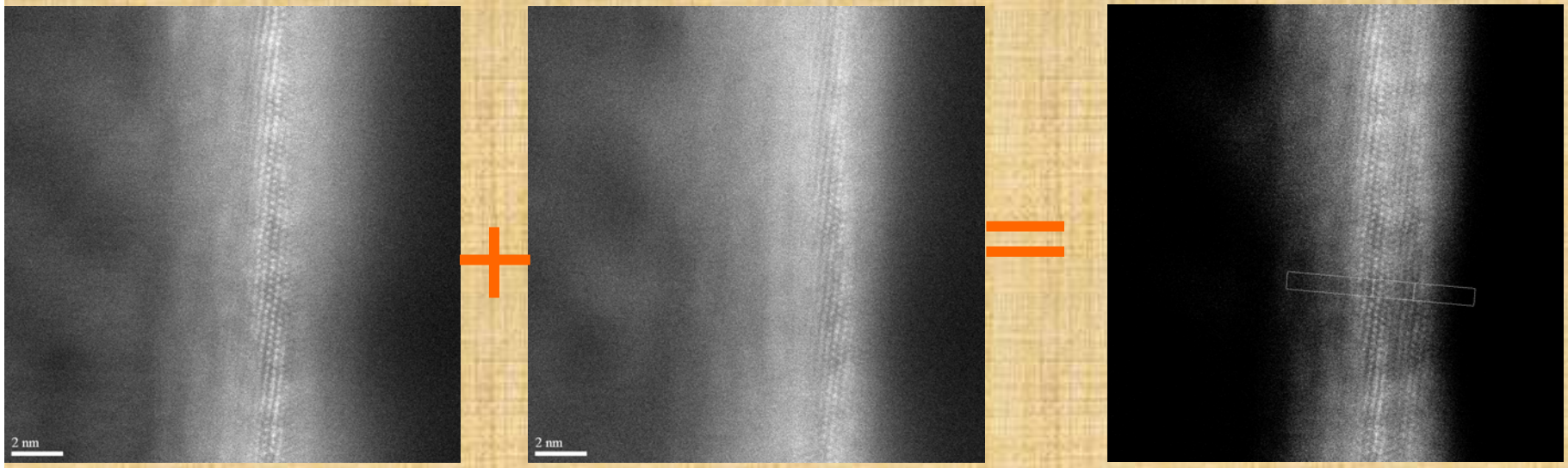
-180nm



-220nm

Through focus image shows the existence of steps. But, how sharp the steps are ?

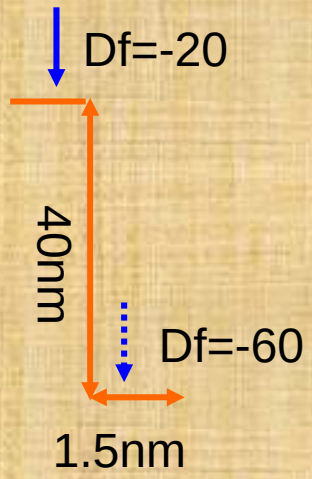
Sharp steps-A through focus study

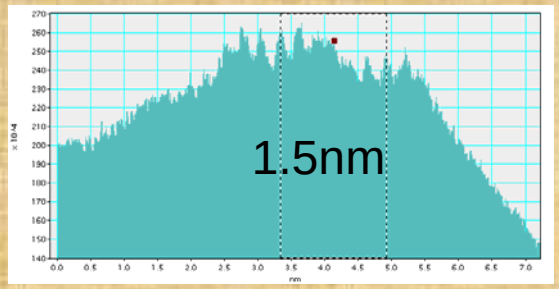


Df=-20nm

Df=-60nm

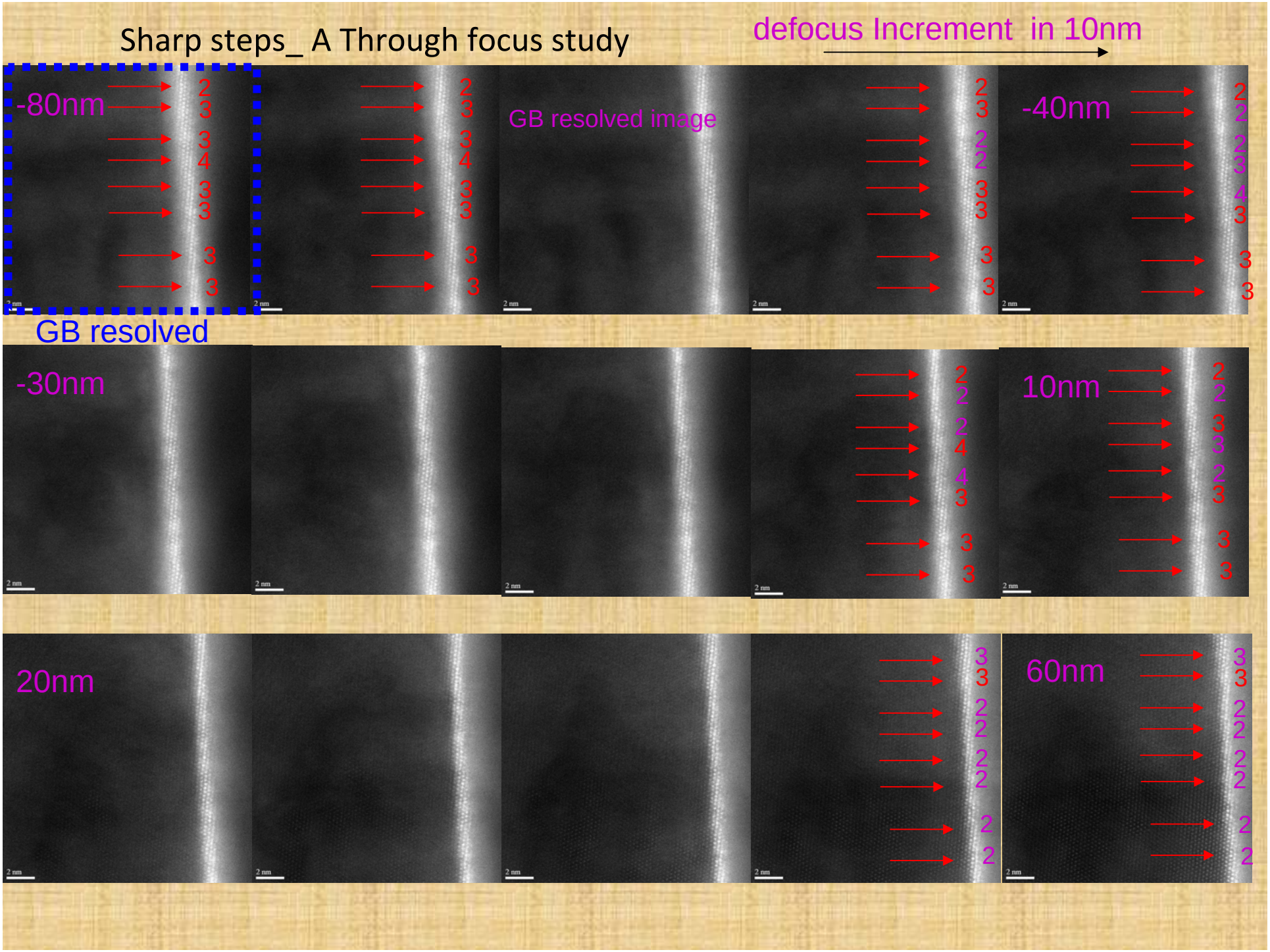
Combined image



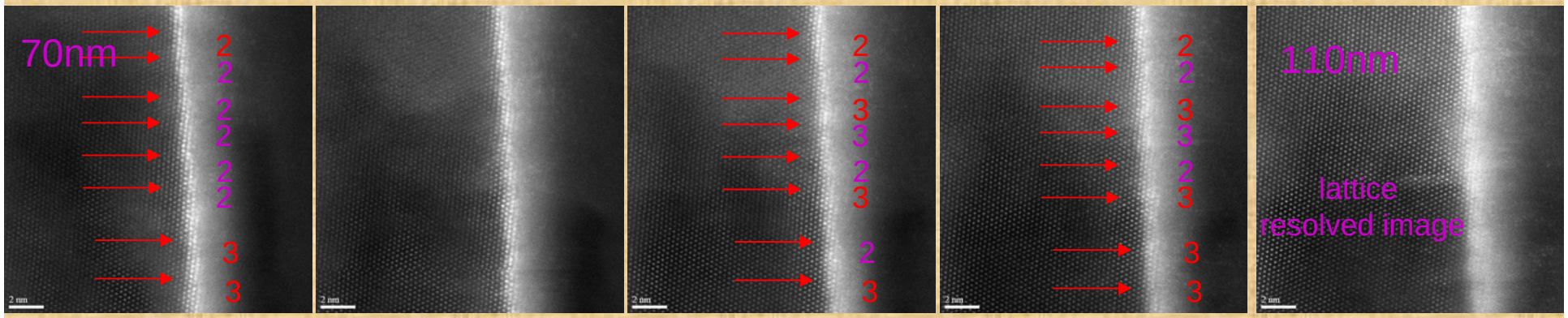


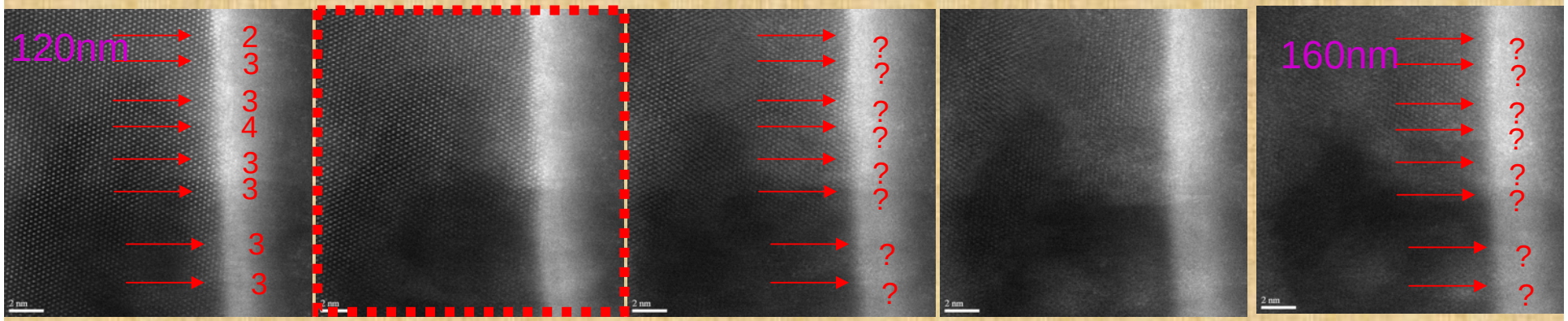
Line profile in the combined image

The slope of the steps could be estimated as 40nm/1.5nm=26


Sharp steps_ A Through focus study
defocus Increment in 10nm
-80nm
GB resolved image
-40nm
GB resolved
-30nm
10nm
20nm
60nm

Continued





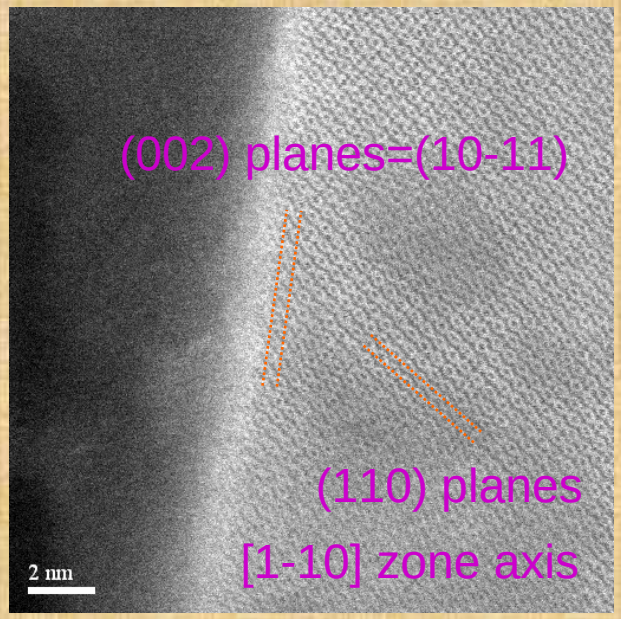
lattice resolved

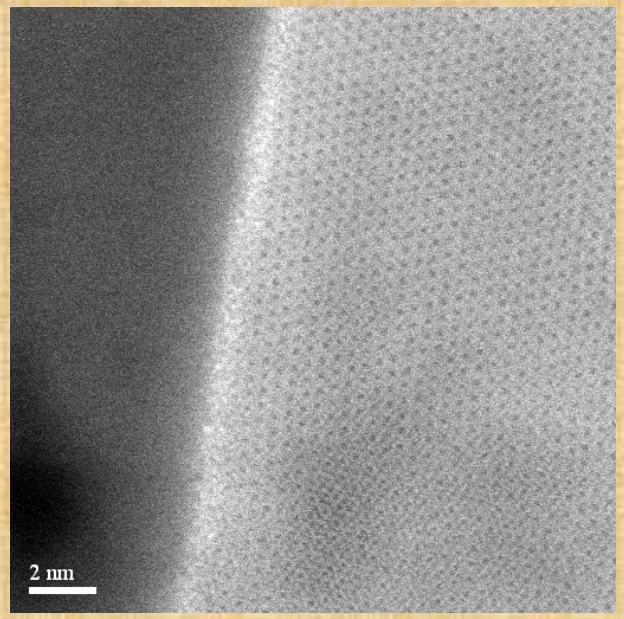
Through focus imaging suggest that GB and crystal matrix are imaged at different defocus values. Sharp atomic level steps is a reasonable explanation.

Further STEM image calculation are under way!

Note: Sample is drifting.

Further study-investigation roles of other dopants





DF=-20nm

DF=-60nm

Yttrium doped sample: Primary results

- Yb, Ba, Hf, La segregation behavior
- Crystal morphology change
- Correlation with oxidation property

Conclusions

- Atomic side faceting is generally observed in Hf-doped alumina sample.
- One atomic height steps are found both in the horizontal planes and in the beam directions!
- It should be admitted that, the substitution of Hf atoms into the Al atoms, which is periodic, should have direct correlation with the improved oxidation behavior of Hf-doped alumina.

Acknowledgements

- Animesh Kundu, Patrick Cantwell, Rob Keyse, and Qian He in Lehigh University for electron microscopy assistance

- Lin Xie in Tsinghua University for STEM image calculation discussion

Thanks for attention!