

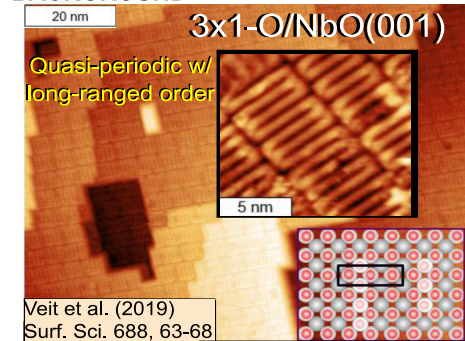


Surface-phonon physics from the semi-dynamical matrix: improved convergence for *ab initio* prediction of Helium atom scattering (HAS) from 3x1-O/NbO(001)

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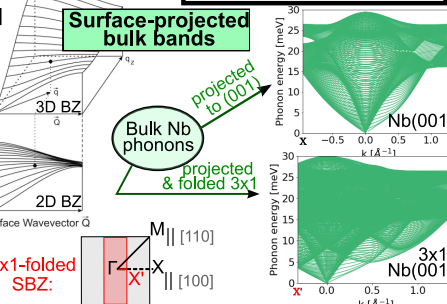


BACKGROUND



monoxide side to study 3x1-O/NbO(001) [top surface]
opportunine model system

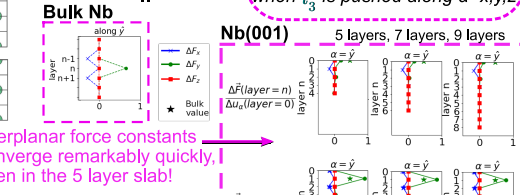
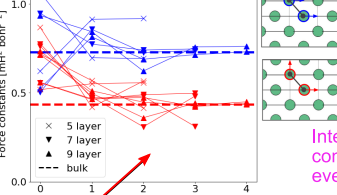
[bottom surface] bare Nb side to test against monatomic Nb(001) slab
3x1-O/NbO(001) consists of a 3-fold ladder-structured monoxide forming on top of BCC Nb(001)



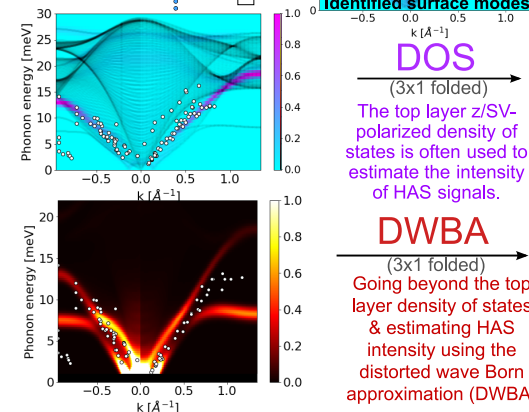
METHODS

$$\sum_{l_1 l_2} \frac{\partial^2 \phi}{\partial u_{l_1}^\alpha \partial u_{l_2}^\beta} \exp [i \mathbf{Q}_{||} \cdot (l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2)] = D_{\alpha\beta} (l_3 \kappa, l_3 \kappa', \mathbf{Q}_{||})$$

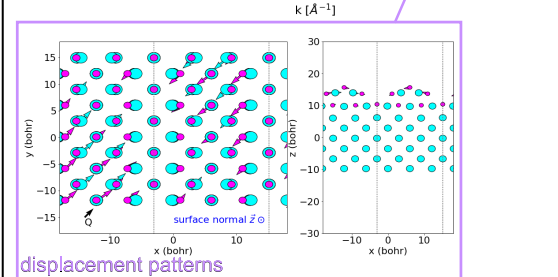
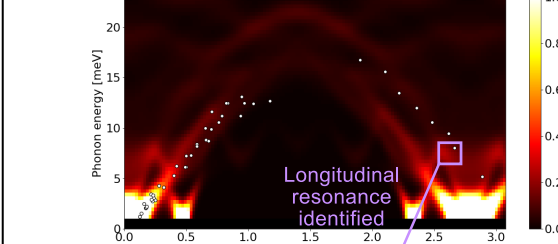
2D Fourier Transform of Force Constant Matrix = 'Semi-Dynamical Matrix' = $\mathbf{Q}_{||}$ -dependent interplanar force constants: the responding force l_3' feels when l_3 is pushed along $\alpha=x,y,z$



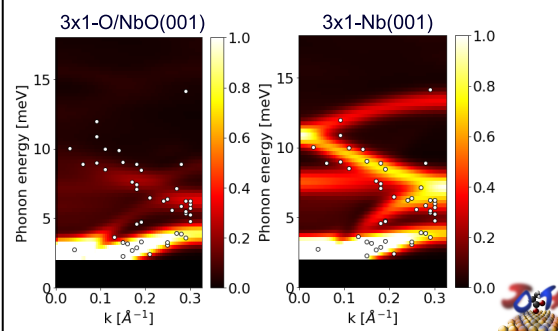
Nearest-neighbor force constants have complicated convergence patterns & 5-layer slab is completely unconverged
Interplanar force constants converge remarkably quickly, even in the 5 layer slab!



3x1-O/NbO(001) RESULTS



Γ X' direction



[X] Benedek & Toennies (2018) Atomic Scale Dynamics at Surfaces