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Title: Principle Vibrational Modes - a New Tool to Visualize the Essence of How Atoms Move in Materials

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Intended for: These slides will serve to document my progress on this project for internal and external colleagues as well as funding agencies.

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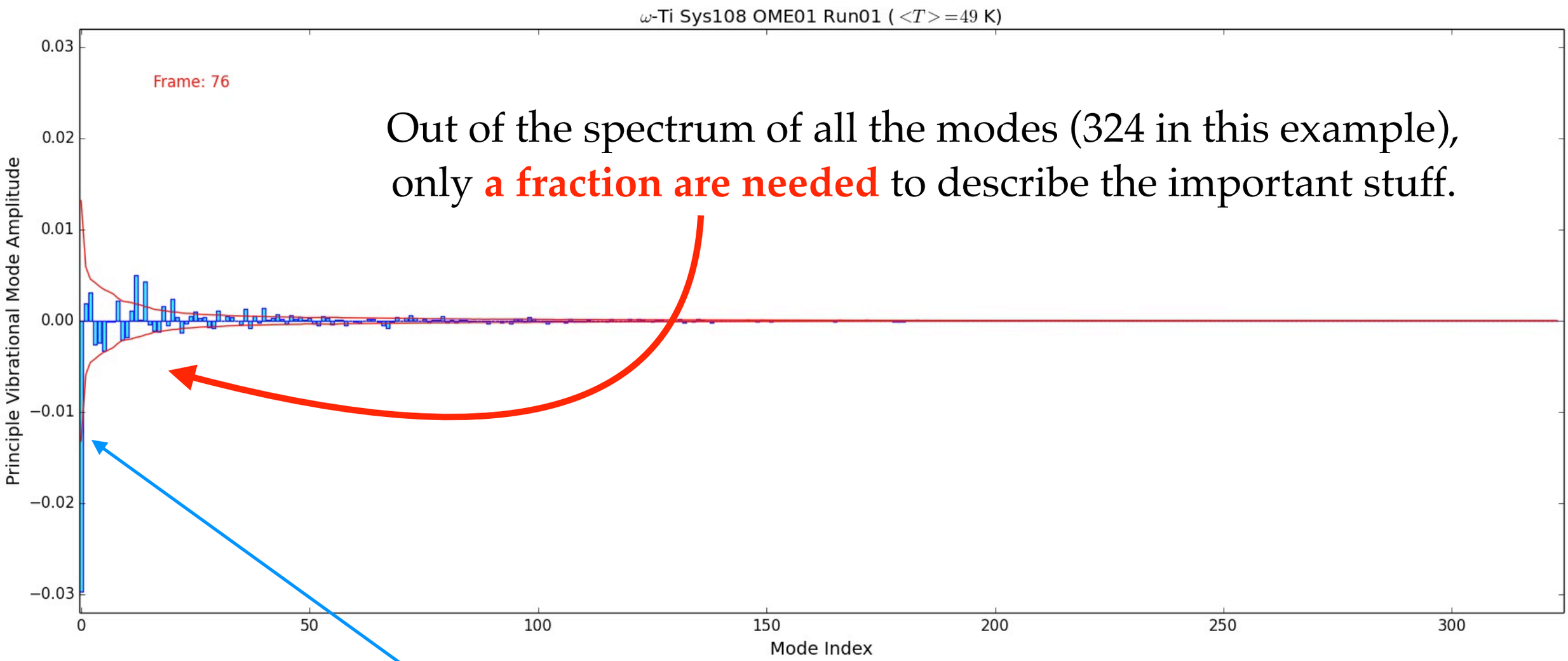
Principle Vibrational Modes

a New Tool to Visualize the Essence of How Atoms Move in Materials

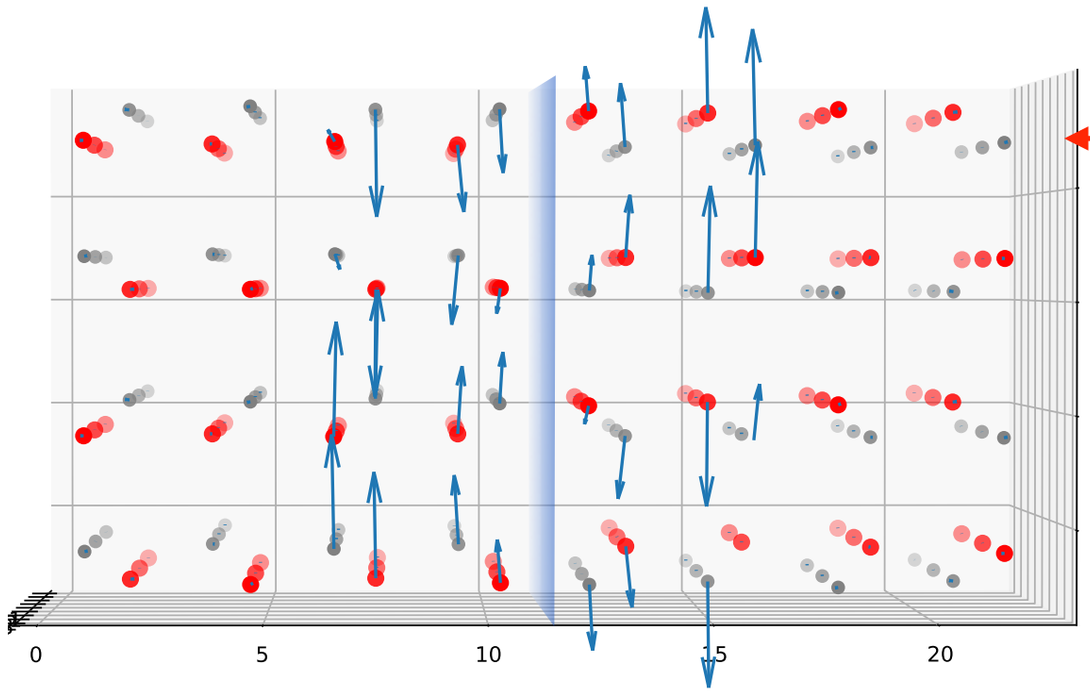
Grouping together the correlated movement of atoms ("rotating the basis") delivers modes with maximum information on the dynamic behavior.



Out of the spectrum of all the modes (324 in this example), only **a fraction are needed** to describe the important stuff.

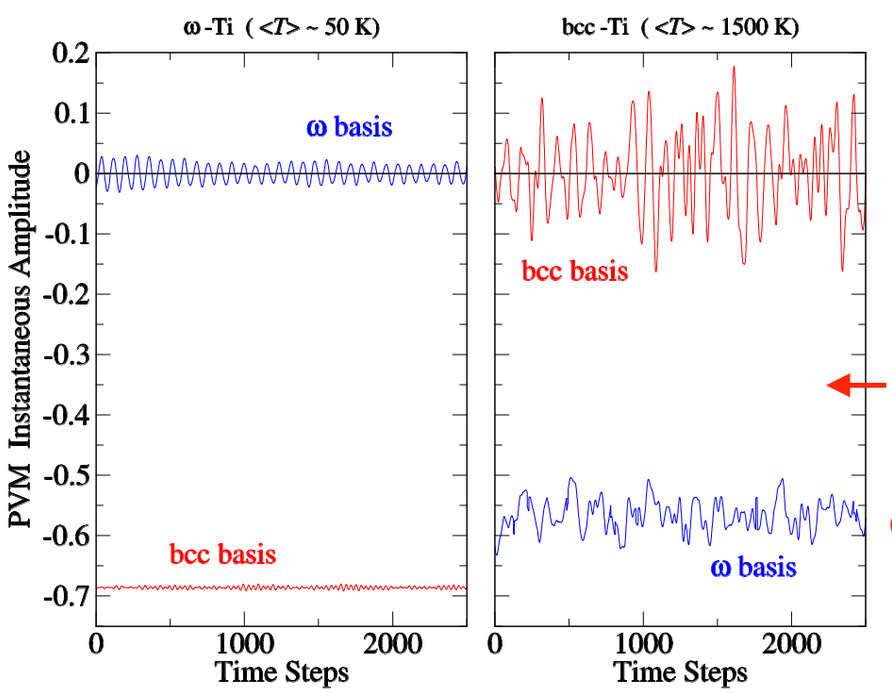
The zeroth mode("PVM_0") dominates and has physical significance…

Three Examples of the Physical Significance of PVM_0



← PVM_0 describes a localized vibration across an inversion domain wall of ZnO.

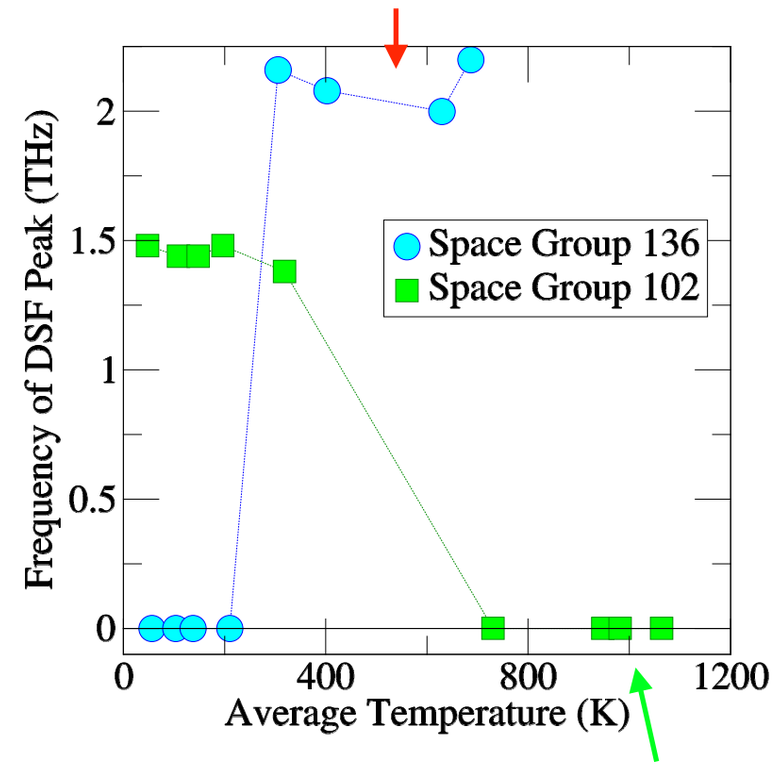
Better understanding of the dynamics at domain walls means better control.



← PVM_0 acts as an order parameter across the ω-bcc structural phase transition of titanium.

At 50 K, Ti vibrates around the ω basis.
At 1500 K, Ti vibrates around the bcc basis.

PVM_0 acts to identify the correct space group for temperature-stabilized beta-Uranium.



At 1000 K, U has moved away from spacegroup 102.