Stress induced inhomogeneous destabilization mechanisms in ideal crystals

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THE STABILITY OF CRYSTAL LATTICES. III

AN ATTEMPT TO CALCULATE THE TENSILE STRENGTH OF A CUBIC LATTICE BY PURELY STATIC CONSIDERATIONS

BY M. BORN AND R. FÜRTH

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the notation
$$F_i = \frac{\partial F}{\partial a_i} \quad \text{and} \quad F_{ij} = \frac{\partial F}{\partial a_i \, \partial a_j}. \tag{7'}$$

Hence instead of (6) we have
$$F = F^0 + \sum_i F_i^0 \delta a_i + \tfrac{1}{2} \sum_i \sum_j F_{ij}^0 \delta a_i \delta a_j + \dots \tag{8}$$

By reasons of symmetry the six quantities F_i^0 reduce to four, so that
$$F_i^0 = (F_1^0, F_2^0, F_2^0, F_4^0, F_5^0, F_5^0), \tag{9}$$
and the thirty-six quantities F_{ij}^0, because of (4), (4′) and (7′), reduce to four, so that
$$(F_{ij}^0) = \begin{pmatrix} F_{11}^0 & F_{12}^0 & F_{12}^0 & 0 & 0 & 0 \\ F_{12}^0 & F_{22}^0 & F_{23}^0 & 0 & 0 & 0 \\ F_{12}^0 & F_{23}^0 & F_{22}^0 & 0 & 0 & 0 \\ 0 & 0 & 0 & F_{23}^0 & 0 & 0 \\ 0 & 0 & 0 & 0 & F_{12}^0 & 0 \\ 0 & 0 & 0 & 0 & 0 & F_{12}^0 \end{pmatrix} \tag{10}$$

and from (15) and (16) the fifth of the conditions (14) follows immediately. Thus, the necessary and sufficient conditions for the stable equilibrium of the lattice are

$$F_{11}^0 > 0, \quad F_{22}^0 > 0, \quad F_{12}^0 > 0, \quad F_{23}^0 > 0, \quad F_{22}^0 - F_{23}^0 > 0, \quad F_{11}^0(F_{22}^0 + F_{23}^0) - 2(F_{12}^0)^2 > 0. \tag{17}$$

$(F_{44} > 0)$ $(F_{55} > 0)$

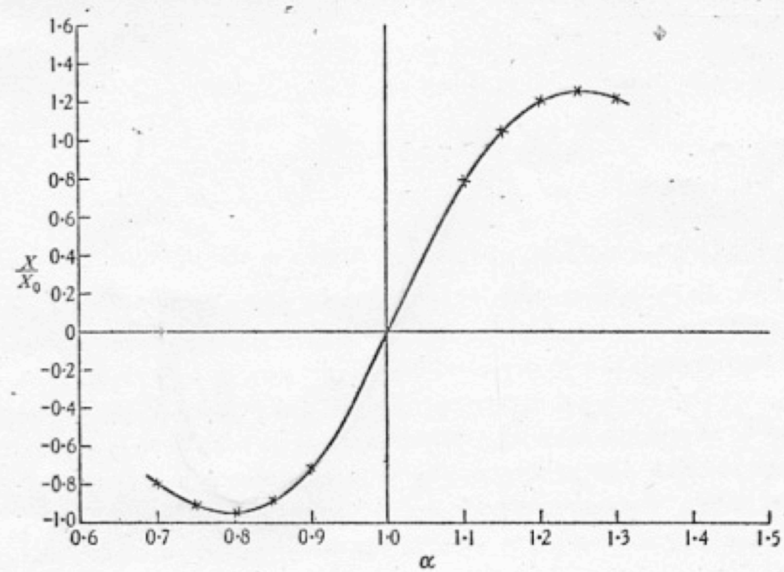

Fig. 1.

The results are contained in table I and the figure. Up to deformations of about 10 % the curve is practically a straight line, i.e. Hooke's law is satisfied. For larger deformations the deviations from Hooke's law increase more and more and, after passing the values $\alpha = 1{\cdot}25$ (or $\alpha = 0{\cdot}8$ for a pressure), X decreases again with and from (15) and (16) the fifth of the conditions (14) follows immediately. Thus, the necessary and sufficient conditions for the stable equilibrium of the lattice are

$$F^0_{11} > 0, \quad F^0_{22} > 0, \quad F^0_{12} > 0, \quad F^0_{23} > 0, \quad F^0_{22} - F^0_{23} > 0, \quad F^0_{11}(F^0_{22} + F^0_{23}) - 2(F^0_{12})^2 > 0. \tag{17}$$

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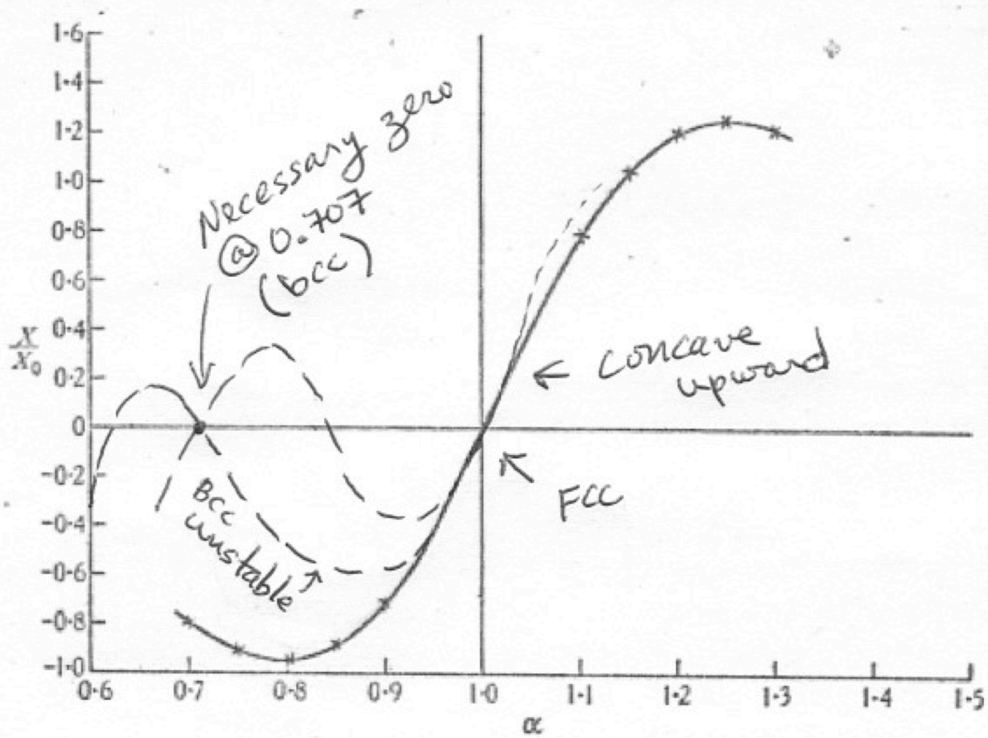

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Consider the [100] loading of an initially cubic crystal. Under uniaxial load ($p_1 \neq 0$, all other $p_r = 0$), the crystal becomes tetragonal on a primary path ($q_1 \neq q_2 = q_3$; cell edges remain perpendicular) with six independent moduli c_{rs}, viz. c_{11}, $c_{12} = c_{13}$, $c_{22} = c_{33}$, c_{23}, c_{44}, and $c_{55} = c_{66}$ (all other $c_{rs} = 0$, and $c_{rs} = c_{sr}$, of course). The differential relations (2) that govern an arbitrary differential disturbance are then

$$\begin{aligned}
dp_1 &= c_{11}\, dq_1 + c_{12}\,(dq_2 + dq_3),\\
dp_2 &= c_{12}\, dq_1 + c_{22}\, dq_2 + c_{23}\, dq_3\,,\\
dp_3 &= c_{12}\, dq_1 + c_{23}\, dq_2 + c_{22}\, dq_3\\
dp_4 &= c_{44}\, dq_4\,, \quad dp_5 = c_{55}\, dq_5, \quad dp_6 = c_{55}\, dq_6\,.
\end{aligned}$$

The quadratic form $c_{rs}\,\delta q_r\,\delta q_s$ may be reduced to the sum of independent squares (Hill and Milstein, 1977)

$$\begin{aligned}
&[c_{11}\,\delta q_1 + c_{12}\,(\delta q_2 + \delta q_3)]^2 / c_{11} + \tfrac{1}{2}(c_{22} + c_{23} - 2c_{12}^2/c_{11})(\delta q_2 + \delta q_3)^2\\
&\quad + \tfrac{1}{2}(c_{22} - c_{23})(\delta q_2 - \delta q_3)^2 + c_{44}\,\delta q_4^2 + c_{55}\,(\delta q_5^2 + \delta q_6^2)
\end{aligned}$$

The determinant of the moduli matrix factors as

$$det(c_{rs}) = (c_{22} - c_{23})[c_{11}(c_{22} + c_{23}) - 2c_{12}{}^2]\, c_{44}\, c_{55}{}^2 .$$

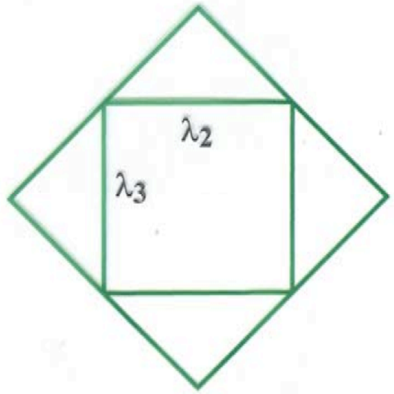
Thus, the necessary and sufficient conditions for Born stability are then

$$c_{11} > 0, \quad c_{22} + c_{23} - 2c_{12}{}^2/c_{11} > 0, \quad c_{22} - c_{23} > 0,$$
$$c_{44} > 0, \quad c_{55} > 0.$$

The determinant can vanish when, and only when, at least one factor does and each vanishing factor is associated with a particular type of eigensolution (Hill and Milstein, 1977):

$$(2c_{12}, -c_{11}, -c_{11}, 0, 0, 0), \text{ when } c_{22} + c_{23} = 2c_{12}{}^2/c_{11},$$
$$(0, 1, -1, 0, 0, 0), \text{ when } c_{22} - c_{23} = 0,$$
$$(0, 0, 0, 1, 0, 0), \text{ when } c_{44} = 0,$$
$$(0, 0, 0, 0, 1, 0) \text{ and } (0, 0, 0, 0, 0, 1), \text{ when } c_{55} = 0.$$

Before branching



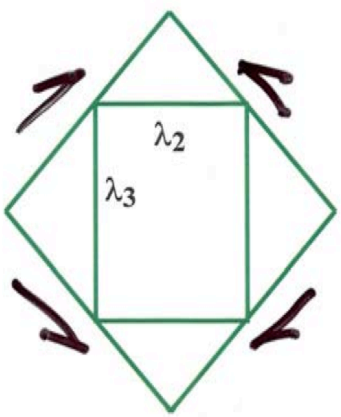
Crystal is tetragonal

$$\lambda_1 \neq \lambda_2 = \lambda_3$$

LOAD IS UNIAXIAL

& NORMAL TO PLANE

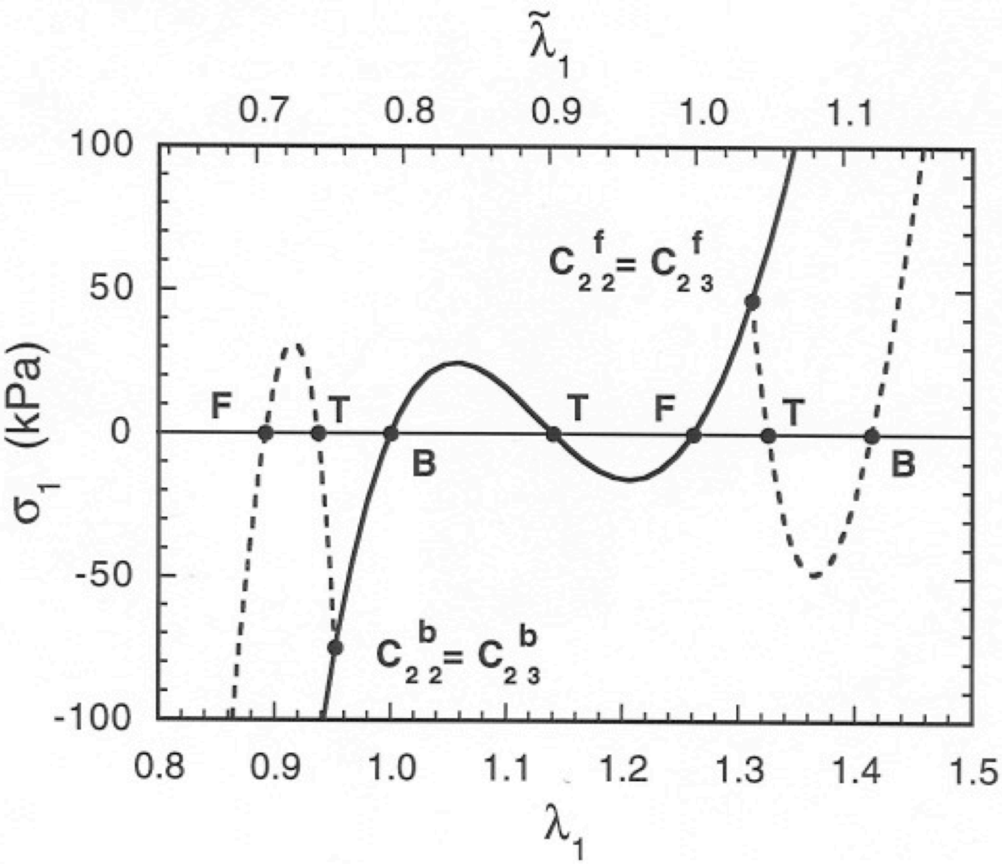
After branching



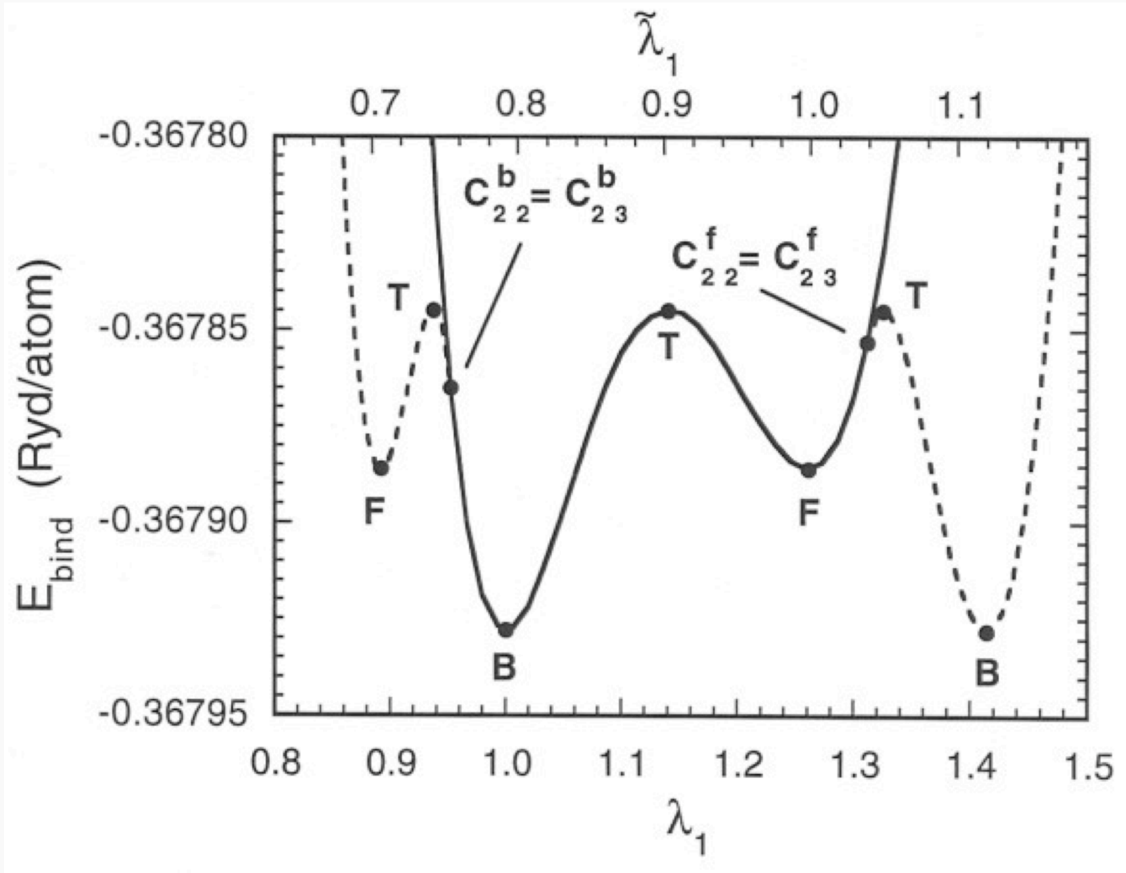
Crystal is orthorhombic

$$\lambda_1 \neq \lambda_2 \neq \lambda_3$$

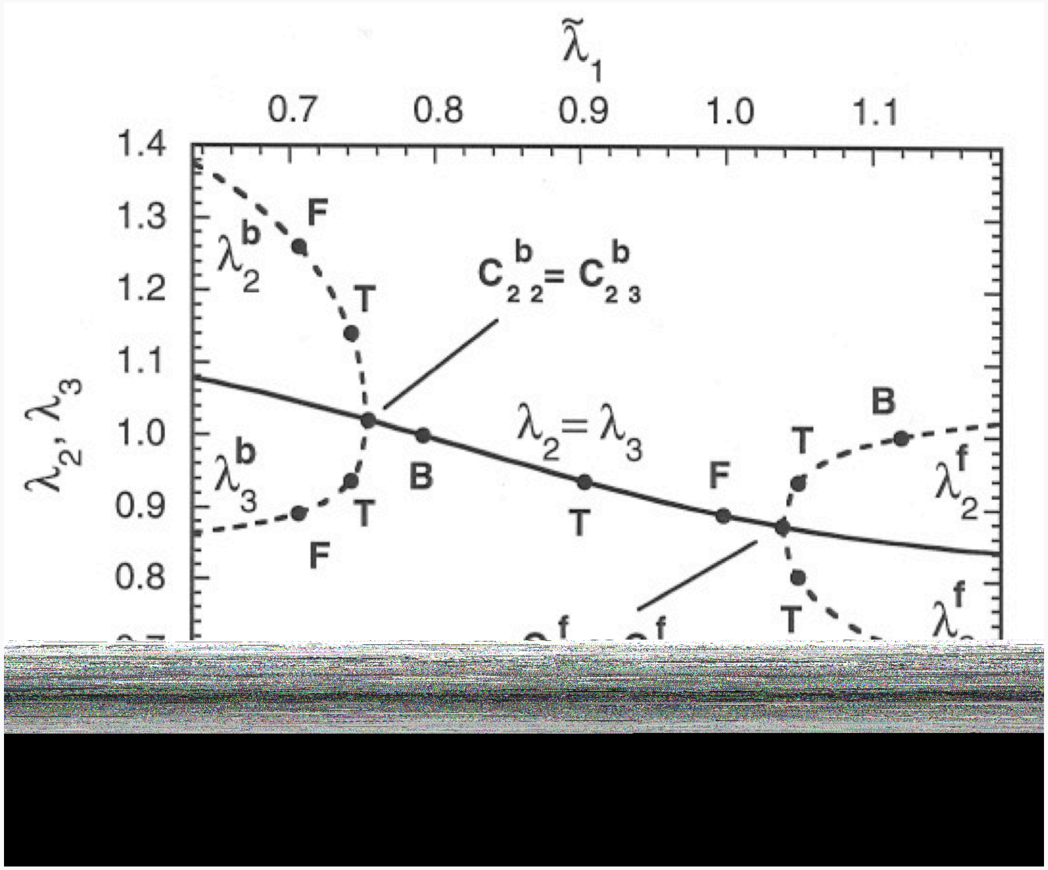
(in general)



F. Milstein, J.Marschall, H.E. Fang, Phys. Rev. Lett. **74**, 2977 (1995)



$\tilde{\lambda}_1$
0.7
0.8
0.9
1.0
1.1
-0.36780
-0.36785
-0.36790
-0.36795
E_{bind} (Ryd/atom)
$C^b_{22} = C^b_{23}$
$C^f_{22} = C^f_{23}$
T
T
T
F
F
B
B
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
λ_1



$\tilde{\lambda}_1$
0.7
0.8
0.9
1.0
1.1
1.4
1.3
1.2
1.1
1.0
0.9
0.8
λ_2, λ_3
λ_2^b
λ_3^b
$C_{22}^b = C_{23}^b$
$\lambda_2 = \lambda_3$
λ_2^f
F
T
B

Computational Methods

Two-step Simulation/Analysis Procedure:

❖ Isostress-Isothermal MD Simulation $(N\underline{\underline{\sigma}}T)$:

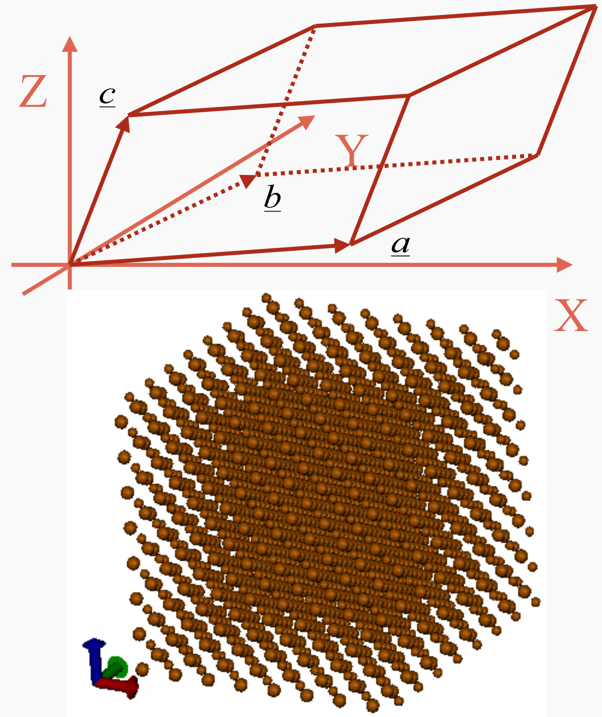
Parrinello-Rahman Lagrangian formulation with additional dynamical variables,

$$\underline{\underline{h}} = [\underline{a}, \quad \underline{b}, \quad \underline{c}]$$

[M. Parrinello and A. Rahman, *J. Appl. Phys*. 52, 7182 (1981)]

❖ Canonical MD Simulation: Computation of elastic moduli employed in assessments of elastic stability using canonical strain fluctuation formulae

[J. R. Ray, *Comp. Phys. Reports* 8, 109 (1988)]



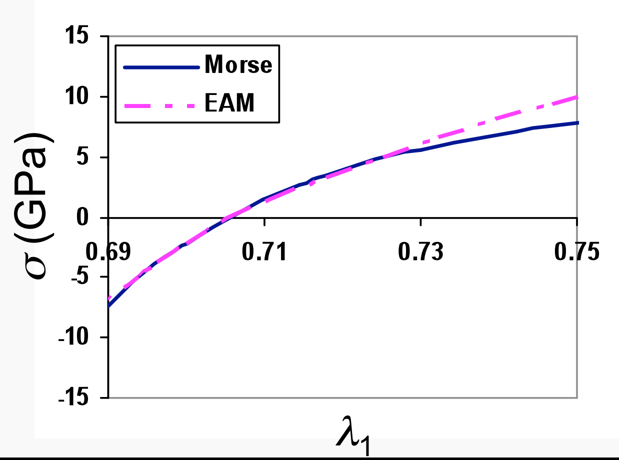
❑ Interatomic interaction described by the

- Morse potential:

$\phi(r) = D\ \{\exp[-2\alpha\,(r-r_0)] - 2\exp[-\alpha\,(r-r_0)]\}$

- EAM potential: $E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_i \sum_{j\neq i} \phi_{ij}(r_{ij})$

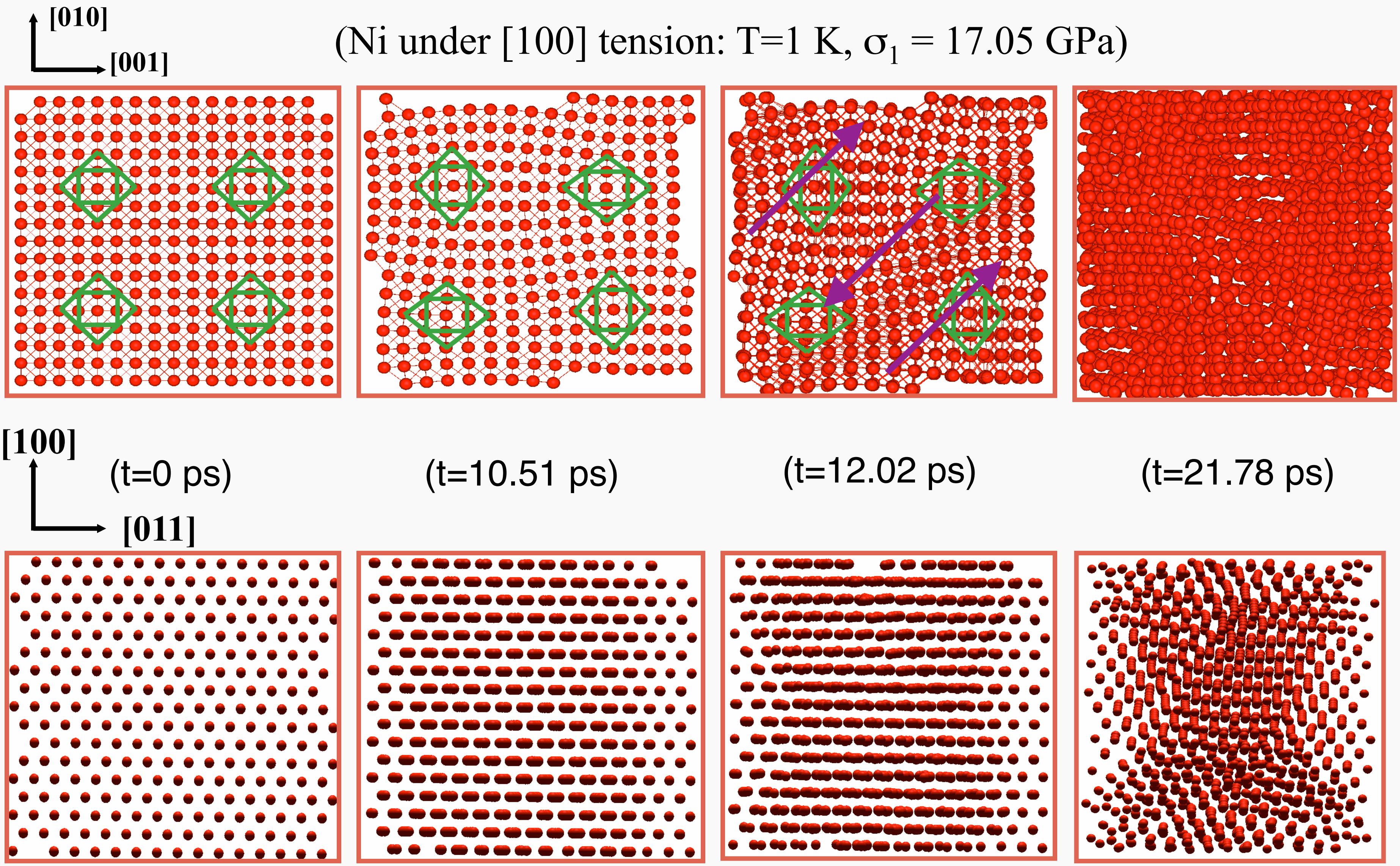
$$\rho_i = \sum_{j\neq i} \rho_j(r_{ij})$$



[S. Chantasiriwan & F. Milstein, *Phys. Rev. B* 58, 5996 (1998); ibid. 58, 6006 (1998); F. Milstein, J. Zhao, and D. Maroudas, *Phys. Rev. B* 70, 184102-1 (2004)]

Response of Morse Ni to Uniaxial [100] Tension: Isostress-Isothermal Molecular Dynamics Simulation

(Ni under [100] tension: T=1 K, σ_1 = 17.05 GPa)



F. Milstein, J. Zhao, and D. Maroudas, Phys. Rev. B, Vol. 70, pp. 1841102 (2004).

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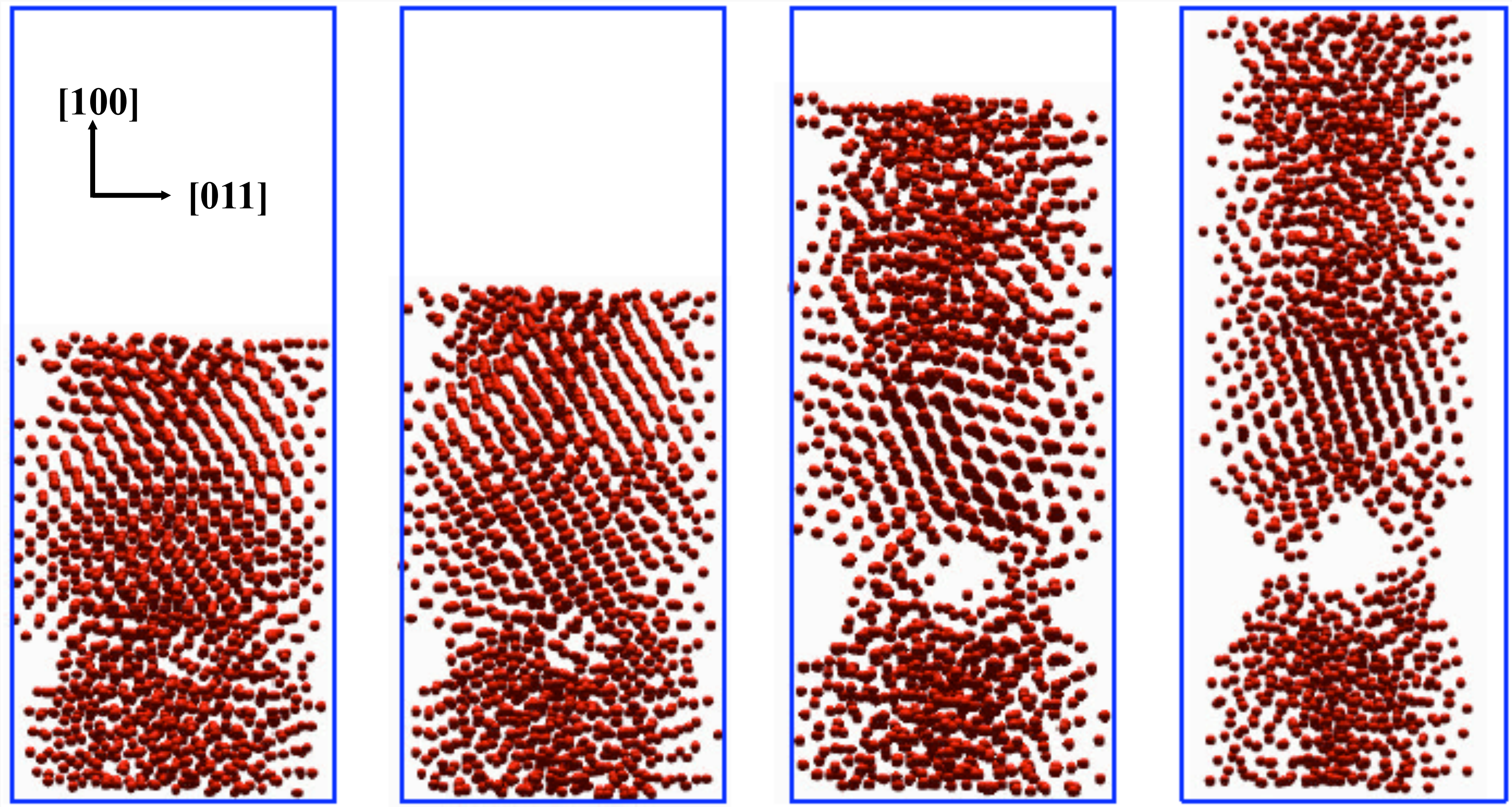
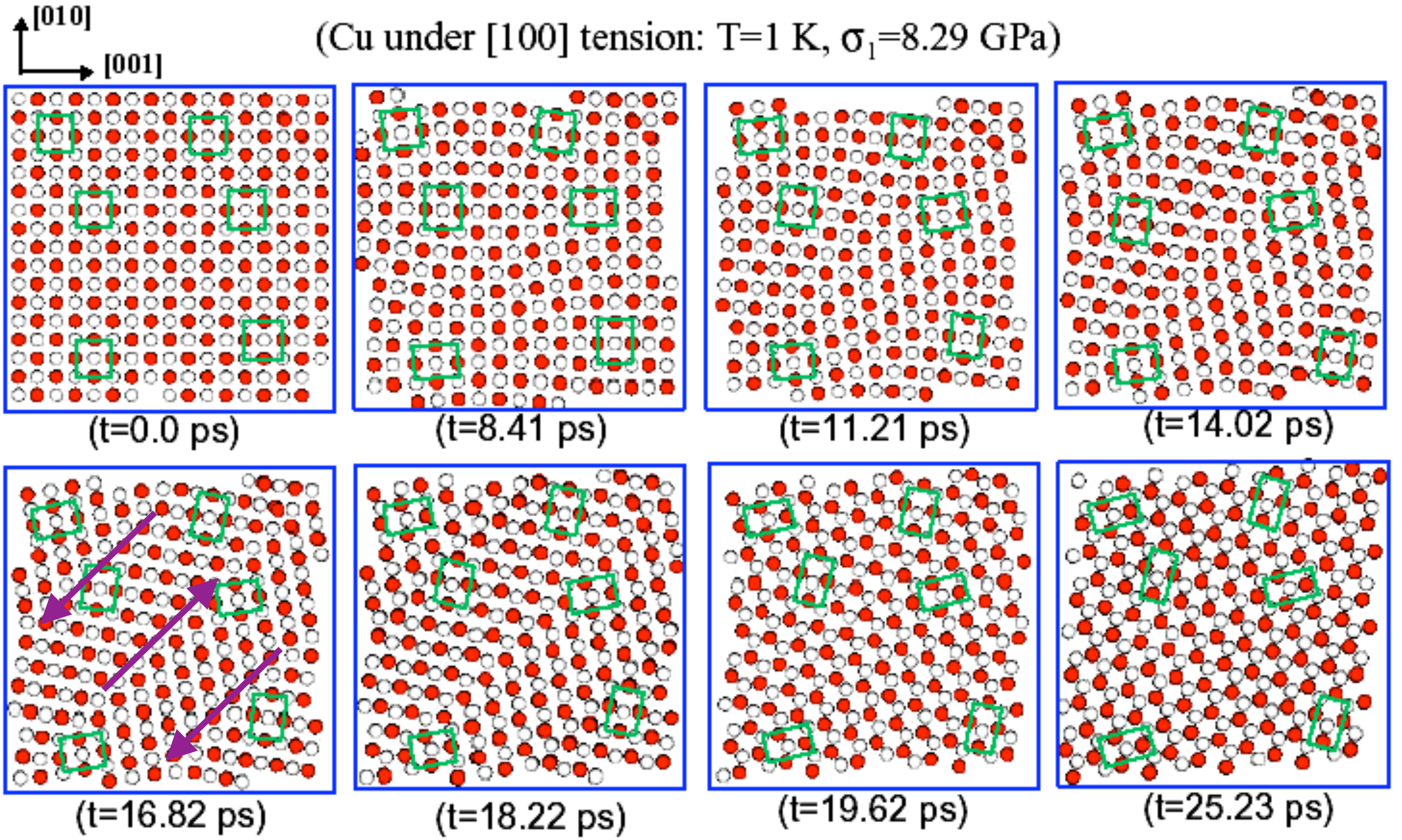


(t=23.28 ps) (t=31.54 ps) (t=42.06 ps) (t=48.06 ps)

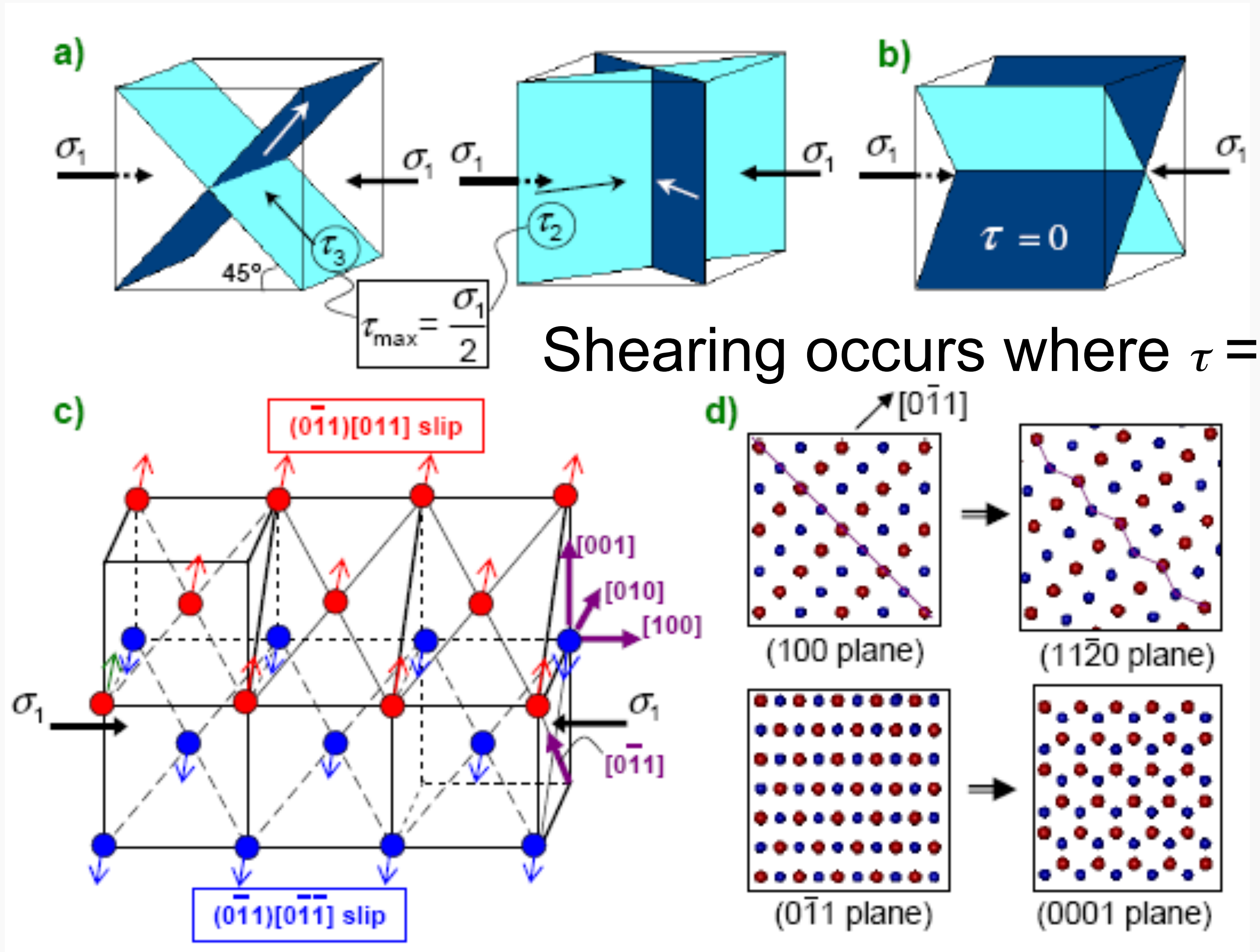
- **Void formation and ultimate failure**

Response of Morse Cu to Uniaxial [100] Tension: Isostress-Isothermal Molecular Dynamics Simulation



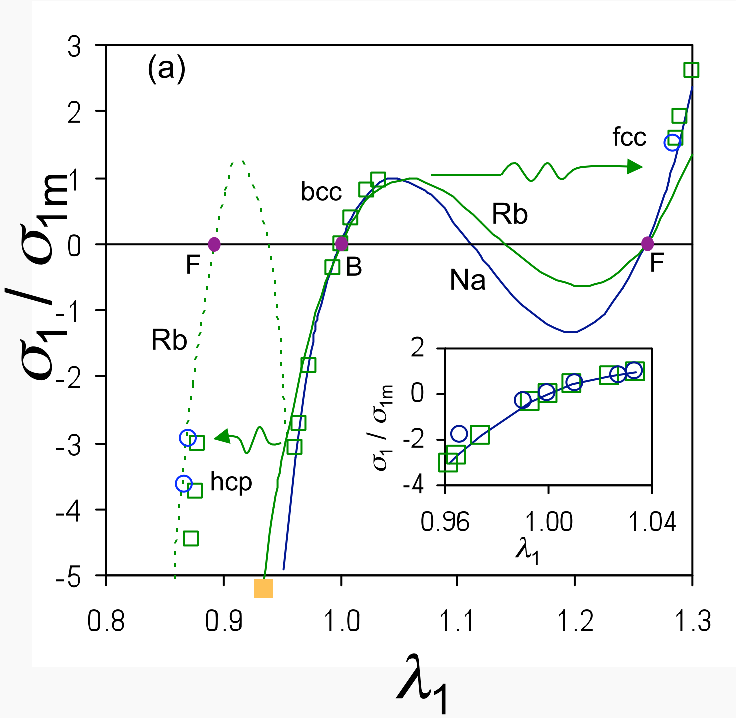
- fcc → hcp structural transformation:
  (100) plane of initial fcc structure → (0001) plane of final hcp structure

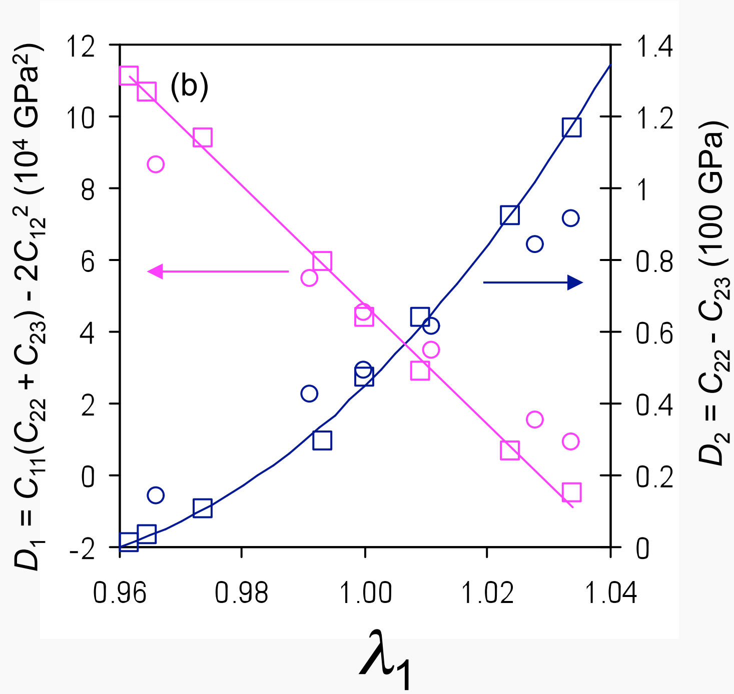
Instability Mechanism of BCC Cu under [100] Uniaxial Compression



Shearing occurs where $\tau = 0$

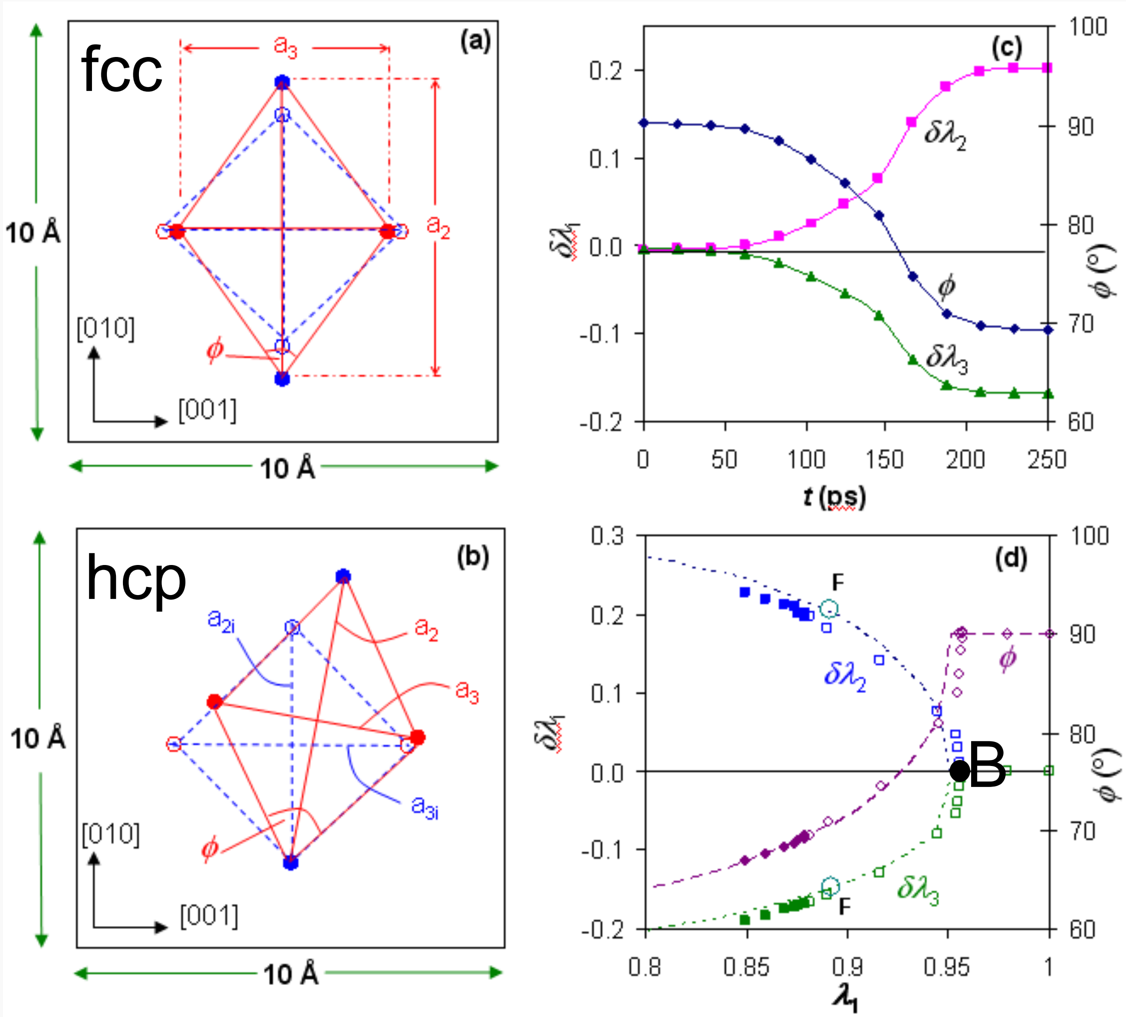
Elastic Stability and Structural Response of BCC K





- The response of bcc K according to the Morse model matches quantitatively the lattice-statics responses of bcc alkali metals (Na - K - Rb) using a quantum mechanically based pseudopotential model
- The bifurcation points obtained from the MD study coincide very well with the ones obtained from the LS pseudopotential calculations (σ_1 / σ_{1m} between -3.0 to -3.3)

Dynamics of BCC-to-HCP Transition



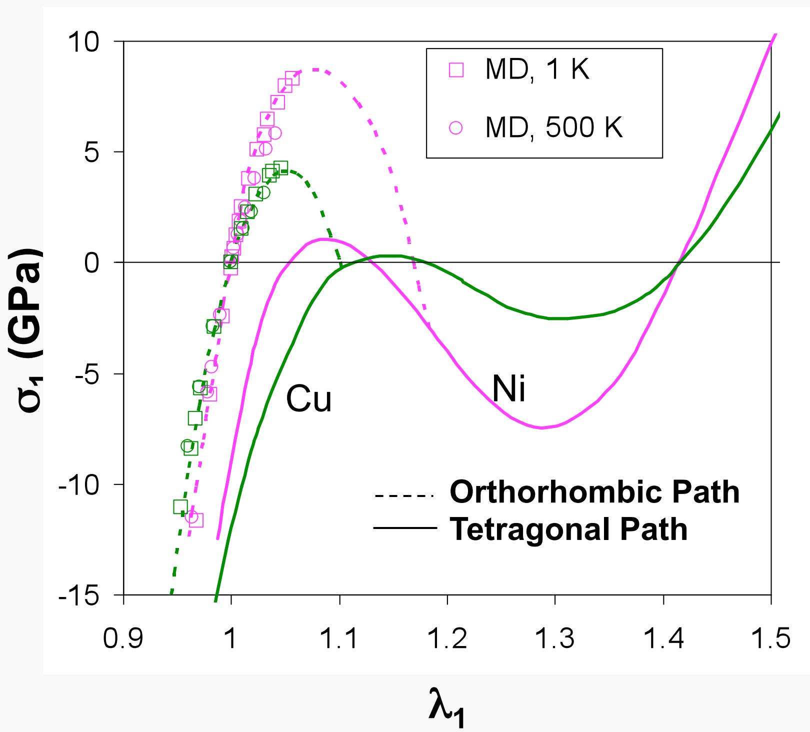
- Comparison between (b) bcc-to-hcp transition observed from MD simulation and (a) bcc-to-fcc transition calculated from pseudopotential model of a bcc alkali crystal
- The lattice stretches, $\delta\lambda_2$ and $\delta\lambda_3$, bifurcate immediately at point B in (d) to either the hcp or the fcc branch; $\delta\lambda_2$, $\delta\lambda_3$, and ϕ show very good agreement between MD simulations and LS pseudopotential calculations.

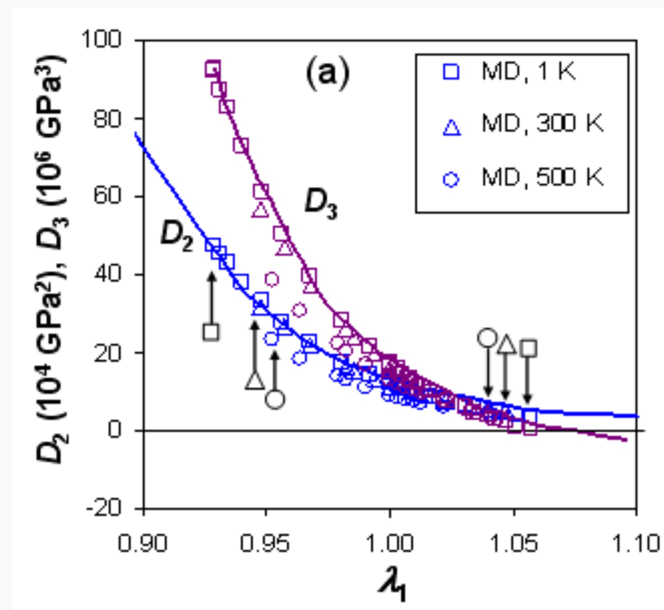
Experimental Findings

- Pressure-induced bcc-to-fcc structural transformation has been observed in the metals: K, Rb, Cs, Ca, Sr, Tl, and Fe
- Pressure-induced bcc-to-hcp structural transformation has been observed in Be, Mg, Ba, Tl, Ti, Zr, and Fe
  [F. Milstein, in *Handbook of Materials Modeling,* edited by S. Yip (Springer, New York, 2005) pp.1223-1279]
- The bcc-to-hcp transition has been observed in many metals as a function of temperature, such as in Zr, or as a function of pressure, such as in Ba, Eu, and Yb
  [Y. Chen, K. M. Ho, and B. N. Harmon, *Phys. Rev. B* **37**, 283 (1988)]
  - Isobaric MD simulations have revealed that temperature increase can induce bcc-to-hcp structural transformations or eliminate simple-cubic-to-hcp transformations
    [J. Zhao, F. Milstein, and D. Maroudas, *Phys. Rev. B* **62**, 13799 (2000); H. Djohari, F. Milstein, and D. Maroudas, *Appl. Phys. Lett*. **90**, 161910 (2007)]
- According to XRD measurements on a K crystal, there is a bcc-to-fcc transition occuring at hydrostatic pressure of 11.6 GPa
  [D. A. Young, *Phase Diagrams of the Elements* (Univ. of California, 1991), p. 62]
- Direct observation of the bcc-to-hcp transition in shock-compressed iron via nanosecond X-ray diffraction at 13 GPa
  [D. H. Kalantar, et al., *Phys. Rev. Lett.* **95**, 075502 (2005)]

  - The MD stability and bifurcation analyses elucidate the similarities and divergences between the bcc-fcc and the bcc-hcp load transitions
    H. Djohari, F. Milstein, and D. Maroudas, Phys. Rev. B, Vol. 79, 174109 (2009).

Structural Response of Morse Ni Crystals to [110] Uniaxial Loading (MD and LS)

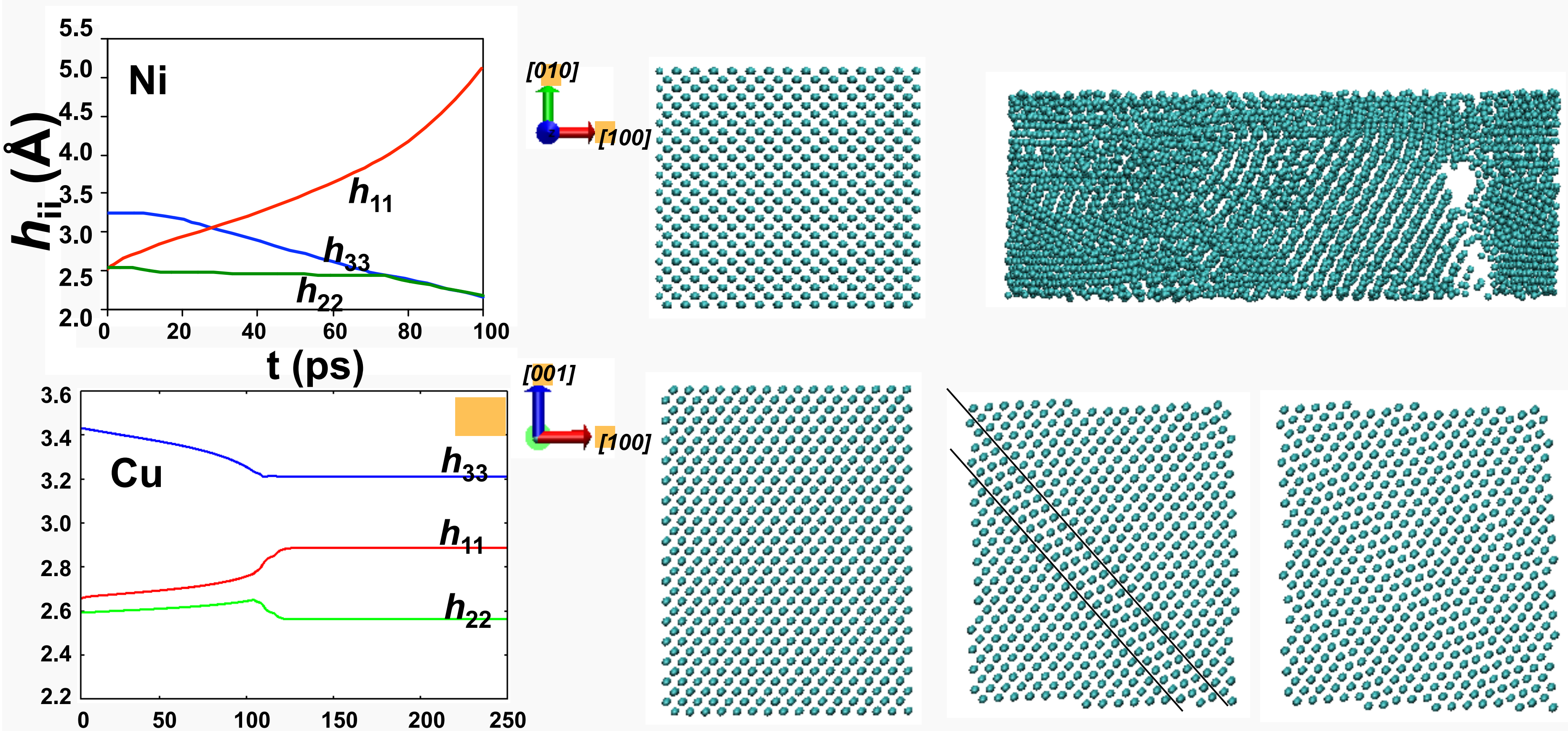




- Instability occurs at or close to the maximum-stress state
- Loss of stability by violating $D_3 > 0$ criterion
- Loss of stability at / close to maximum-stress state is different from instability onset under [100] and [111] loading

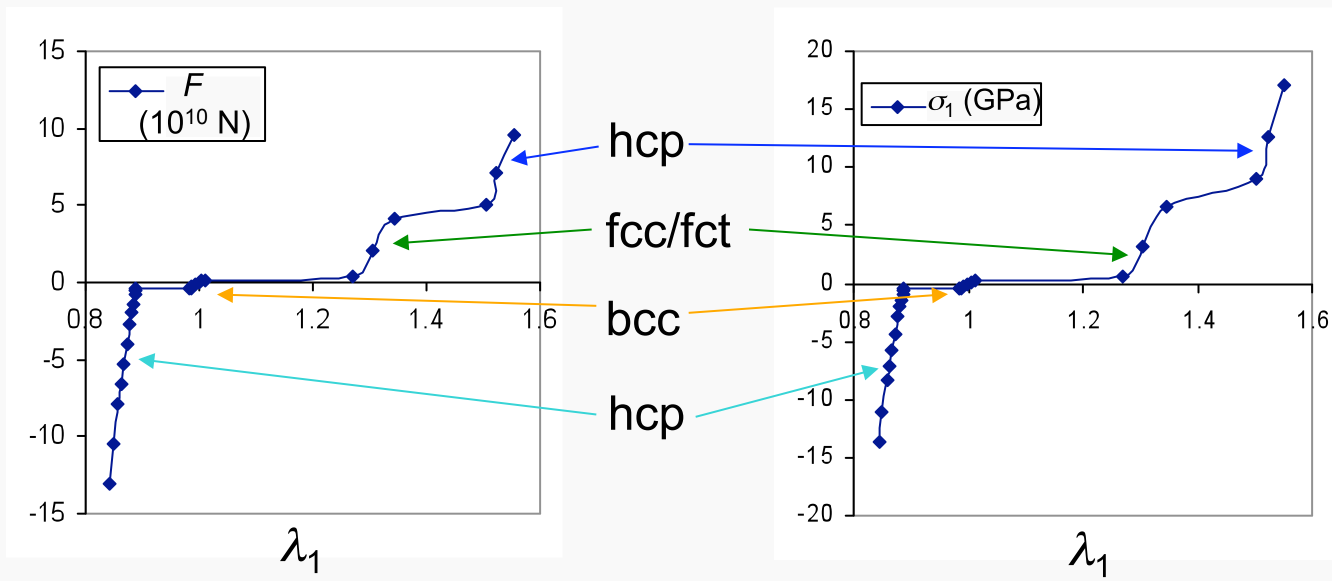
H. Djohari, F. Milstein, and D. Maroudas, Appl. Phys. Lett. **89**, 181907 (2006)

Response of Morse Fcc Ni and Cu to Uniaxial [1 1 0] Tensile Loading



- In Morse Ni, instability triggers the failure of the material
- In Morse Cu, instability leads to slip and formation of stacking faults

Uniaxial Loading Force and Stress during Transformation of Bcc Cu Crystals



- Uniaxial loading force and stress correlate well with each other
- The “gap” in the graph indicates that a transformation occurs

Djohari, Maroudas and Milstein, to be published

Finally consider the notional stability criteria and associated bifurcation response for cubic crystals under [111] uniaxial loading, following the exposition of Milstein, Hill, and Huang (1980). Under [111] loading, the primary path is axisymmetric. Crystal symmetry reduces the number of independent moduli to six, which, together with their interrelationships, are $c_{11} = c_{22}$, c_{33}, $c_{44} = c_{55}$, c_{12}, $c_{13} = c_{23}$, and $c_{14} = -c_{24} = c_{56}$, with $c_{66} = ½(c_{11} - c_{12})$.

The quadratic form $c_{rs}\, \delta q_r\, \delta q_s$ can be arranged as

$$
\begin{aligned}
&[c_{33}\,\delta q_3 + c_{13}\,(\delta q_1 + \delta q_2)]^2 / c_{33} \;+\; [c_{44}\,\delta q_4 + c_{14}\,(\delta q_1 - \delta q_2)]^2 / c_{44} \\
&\quad + ½(c_{11} + c_{12} - 2c_{13}^2/c_{33})(\delta q_1 + \delta q_2)^2 \;+\; ½(c_{11} - c_{12} - 2c_{14}^2/c_{44})[(\delta q_1 - \delta q_2)^2 + \delta q_6^2] \\
&\quad + (c_{44}\,\delta q_5 + c_{14}\,\delta q_6)^2 / c_{44}
\end{aligned}
$$

by successively "completing the square" in the variables taken in a sequence appropriate to the symmetries. The necessary and sufficient conditions for positive definiteness of the quadratic form $c_{rs}\, \delta q_r\, \delta q_s$ under [111] loading, are then

$$(c_{11} + c_{12})\, c_{33} > 2c_{13}^2 \quad \text{and} \quad (c_{11} - c_{12})\, c_{44} > 2c_{14}^2$$

with

$$c_{33} > 0 \quad \text{and} \quad c_{44} > 0.$$

Likewise, factorization of the determinant of the matrix c_{rs} yields

$$det(c_{rs}) = \tfrac{1}{2}[(c_{11} + c_{12})\, c_{33} - 2c_{13}^2]\, [(c_{11} - c_{12})\, c_{44} - 2c_{14}^2]^2.$$

The first factor vanishes at an extremum of p_3 on the primary path, and the eigenmode is that of the axisymmetric path itself; i.e., a first order increment δq_r that does not vary from the primary path is governed by

$$\delta p_3 = [c_{33} - 2c_{13}^2/(c_{11} + c_{12})]\delta q_3\,,$$

with

$$\delta q_1 = \delta q_2 = -\delta q_3\, c_{13}/(c_{11} + c_{12})\,,$$

all other $\delta q_r = 0$. When δp_3 vanishes, the eigenmode becomes

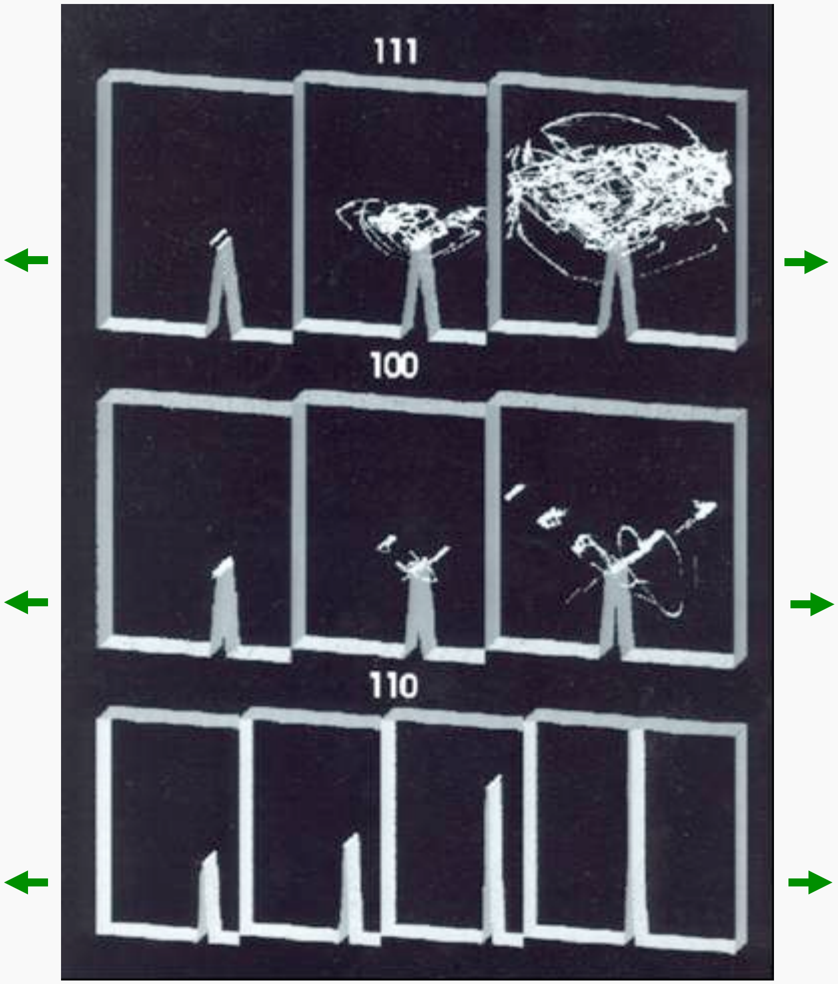
$$\delta q_1 = \delta q_2 = -\delta q_3\, c_{33} / 2c_{13}\,.$$

Vanishing of the second factor, since double, is associated with a pair of independent eigenmodes:

$$\delta q_1/c_{44} = -\delta q_2/c_{44} = -\delta q_4/2c_{14}\,,$$
$$\delta q_5/c_{14} = -\delta q_6/c_{44}\,,$$

all other $\delta q_r = 0$ in both cases.

Connections with
Crack Propagation under Rapid Tensile Loading



- Abraham and coworkers modeled crack propagation under rapid [100], [110], and [111] uniaxial tensile loading of fcc crystals (with Lennard-Jones interactions)
- [111]: Tangled arrays of dislocations consistent with a pair of complex eigenmodes
- [100]: Propagation of individual dislocations at 45° to the loading axis consistent with shearing eigenmode at $c_{22} = c_{23}$
- [110]: Brittle failure (no dislocation emission from the crack tip), consistent with the crystal remaining stable up to a stress level very close to the maximum stress exhibited on the stress-strain curve

F.F. Abraham, and J.Q. Broughton, Comp. Mat. Sci. **10**, 1 (1998)