Introduction to ab initio calculation and κ-carbide

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Pt-group meeting presentation

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First-principles (*ab initio*) caculation

$$\hat{H}\Psi = E\Psi$$

$$\hat{H}\Psi = E\Psi$$ Schrödinger Equation

Ground state energy for any given compound or solid

Variational principle

$$E = \min_{\phi} < \phi|\hat{H}|\phi >, \int_{-\infty}^{\infty} dx|\phi(x)|^2 = 1$$

$$\hat{H}\Psi = E\Psi$$ Schrödinger Equation

Ground state energy for any given compound or solid

$$\{\sum_{i=1}^{n} -\frac{1}{2}\nabla_i^2 + \sum_{i=1}^{n} v_{ex}(r_i) + \sum_{i=1}^{n} v_{ext}(r_i)\}\Psi(r_1, r_2, \ldots, r_n)$$

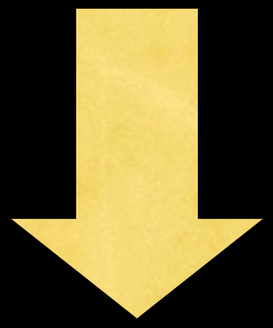
$$= E\Psi(r_1, r_2, \ldots, r_n)$$

Where, $e^2 = \hbar = m_e = 1$

Density Functional Theory (DFT)

$$\{\sum_{i=1}^{n} -\frac{1}{2}\nabla_i^2 + \sum_{i=1}^{n} v_{ex}(r_i) + \sum_{i=1}^{n} v_{ext}(r_i)\}\Psi(r_1, r_2, \ldots, r_n)$$

$$= E\Psi(r_1, r_2, \ldots, r_n)$$



$$\{-\frac{\nabla^2}{4} + \frac{|\nabla n|^2}{8n^2} + v(\mathbf{r})\}n(\mathbf{r}) = En(\mathbf{r})$$

DFT Implementations

- self-consistent
- Harris functional
  - all-electron full potential
  - all-electron muffin-tin
  - all-electron PAW
  - pseudopotential
    - beyond LDA
      - GW
      - model GW
      - sX-LDA
      - time-dependent DFT
      - optimized effective potentials (OEP)
      - LDA+U
      - self-interaction corrections (SIC)
    - generalized gradient approximations (GGA)
    - local density approximation (LDA)

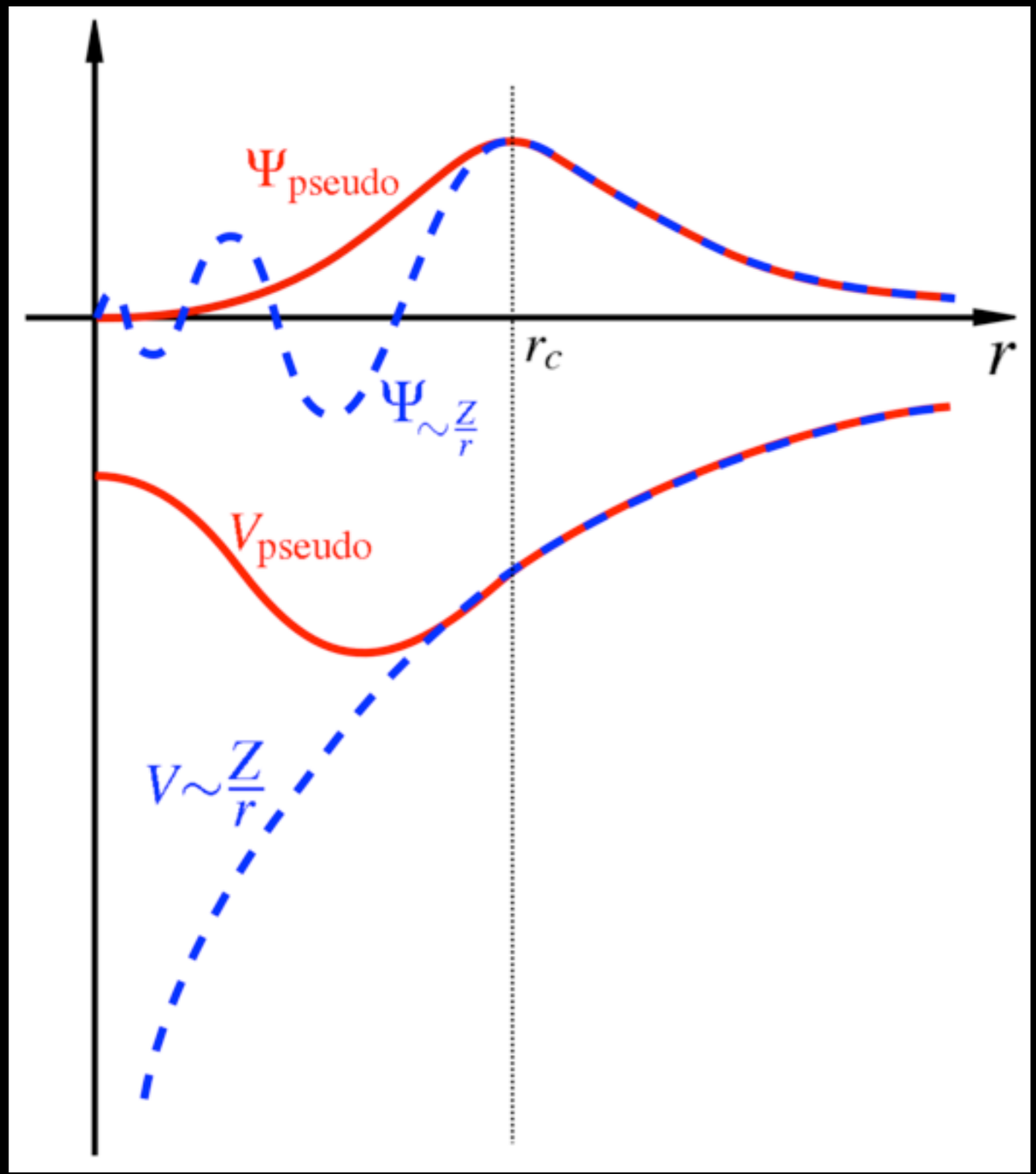
- fully-relativistic
- semi-relativistic
- non-relativistic

$$\left[-\tfrac{1}{2}\nabla^2 + V(\mathbf{r}) + \mu_{xc}(\mathbf{r})\right]\psi_i^k = \varepsilon_i^k \psi_i^k$$

- non-periodic
- periodic
- symmetry

- non-spin-polarized
- spin-polarized

- atomic orbitals
  - Gaussians (GTO)
  - Slater type (STO)
  - numerical (DMol, Siesta)
- plane waves
- augmentation
  - plane waves (FLAPW)
  - spherical waves (LMTO, ASW)
- fully numerical


Ψ_{pseudo}
r_c
r
$\Psi_{\sim\frac{Z}{r}}$
V_{pseudo}
$V\sim\frac{Z}{r}$

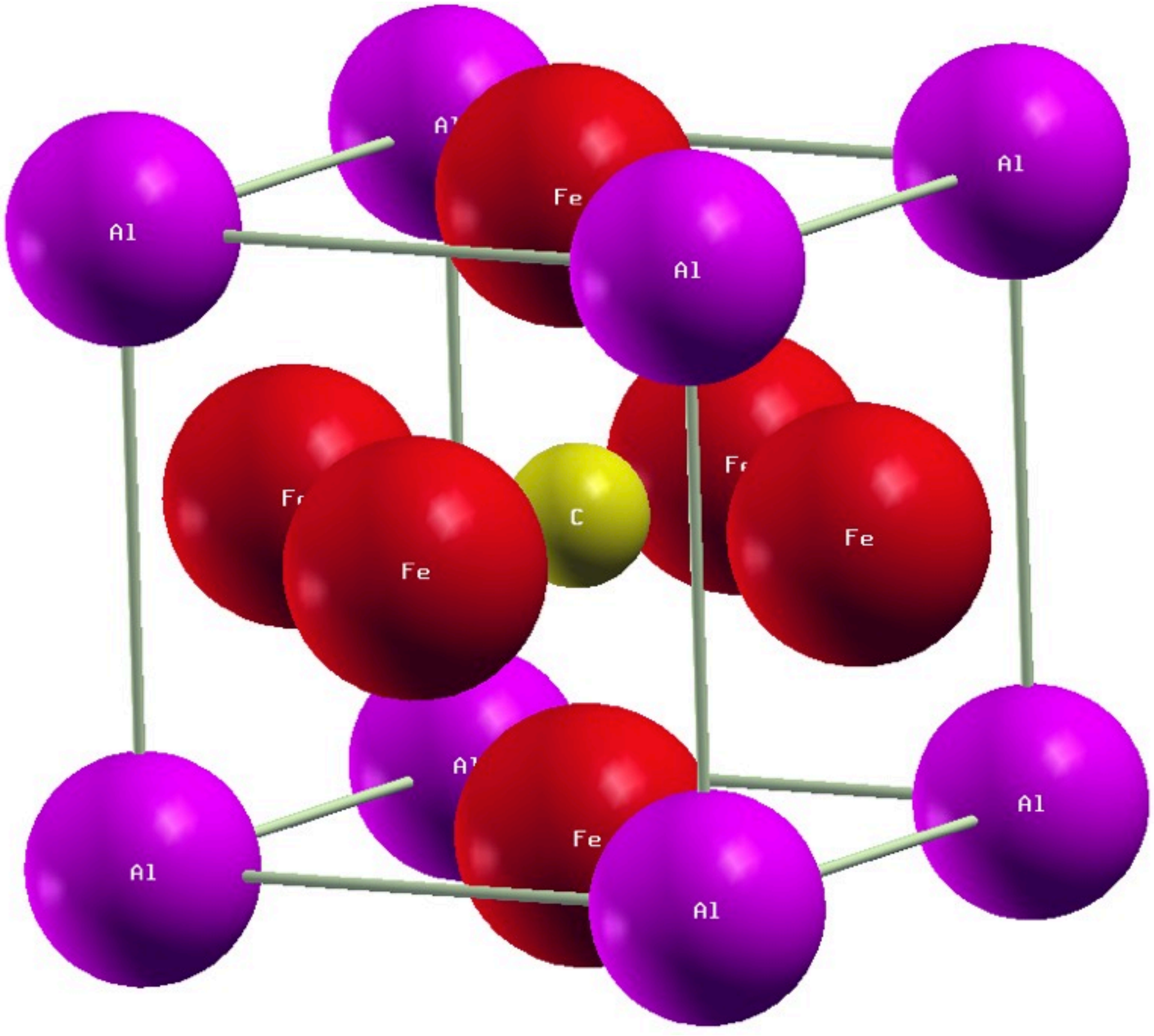
Strong point

- Calculation at 0K is accurate (by theory).
- Making system is easy.
- Magnetic and electric properties.
- It can give thermodynamic variable.

Limitation

- It only calculate ground energy (0K).
- System size is small.
- Computer is too slow.

κ-carbide



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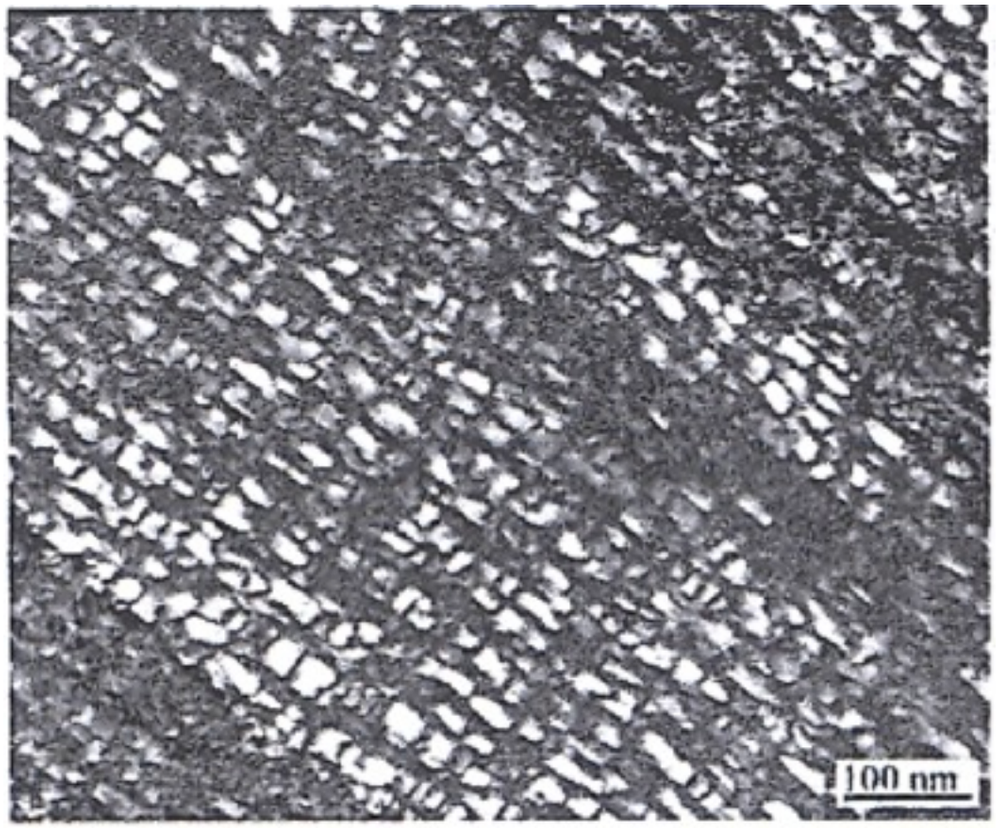


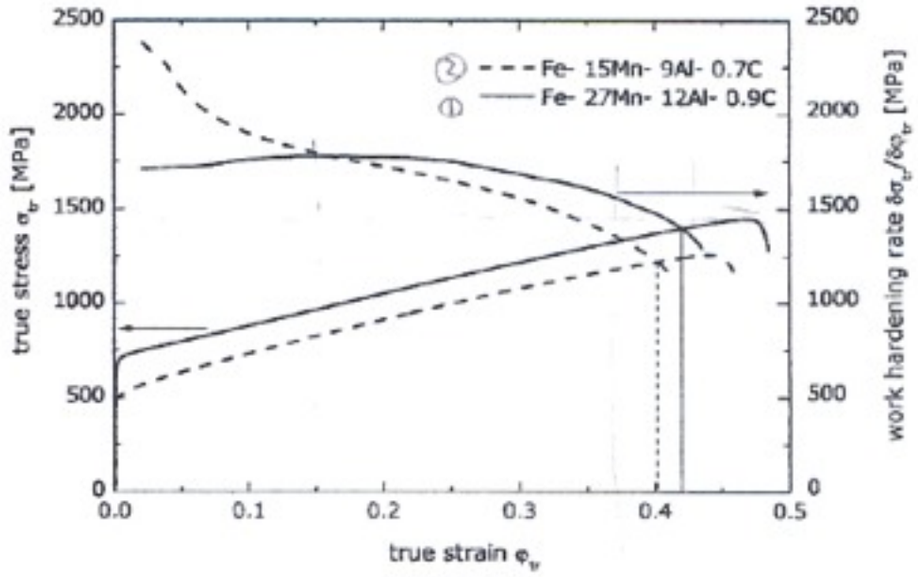


Figure 5. True-stress 'σ_{tr}' as a function of true-strain 'φ_{tr}' and the related work hardening rate $\delta\sigma_{tr}/\delta\varphi_{tr}$ curves of two selected high-manganese-aluminium-carbon steels are showing that Considère's criterion is fulfilled for large plastic strains of about $\varphi_{tr} \approx 0.42$.

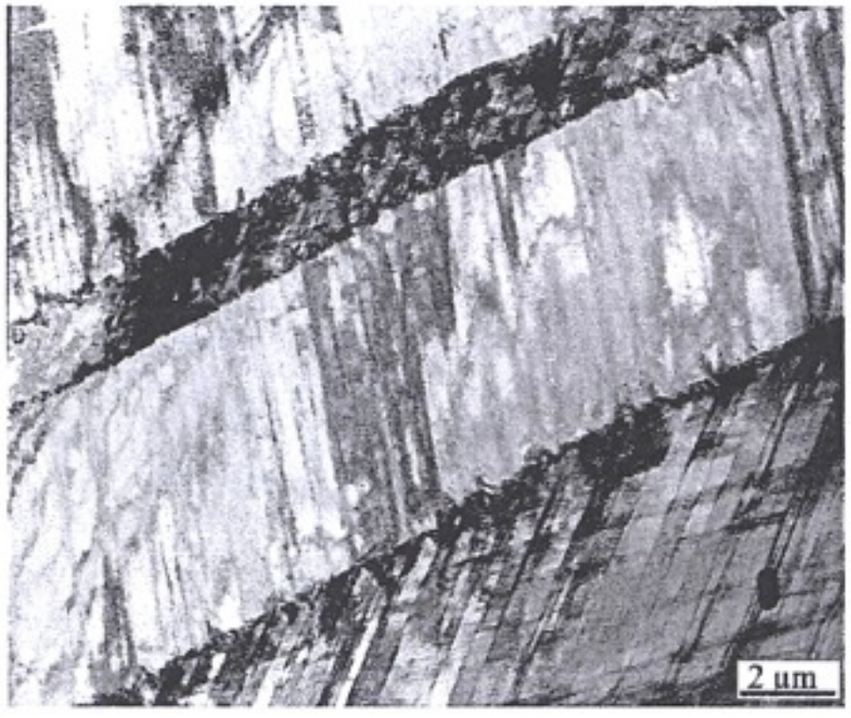


Figure 8a. TEM bright-field image exhibits shear bands on {111} planes in the austenitic matrix.

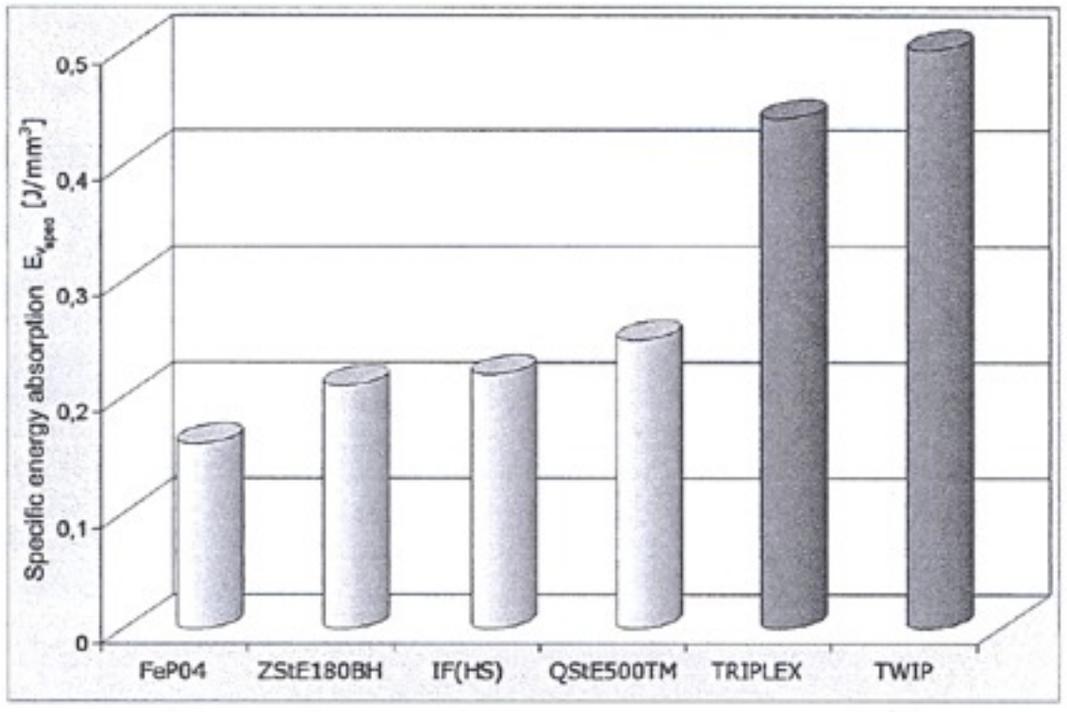
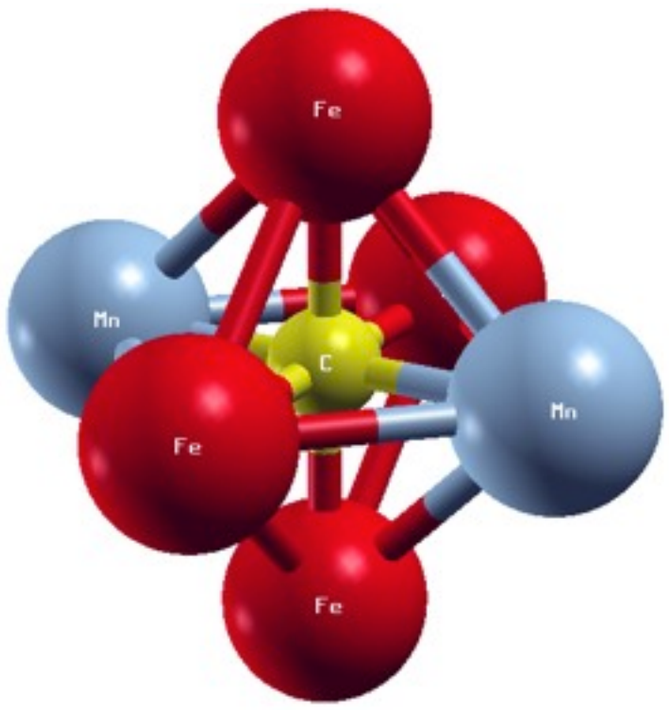
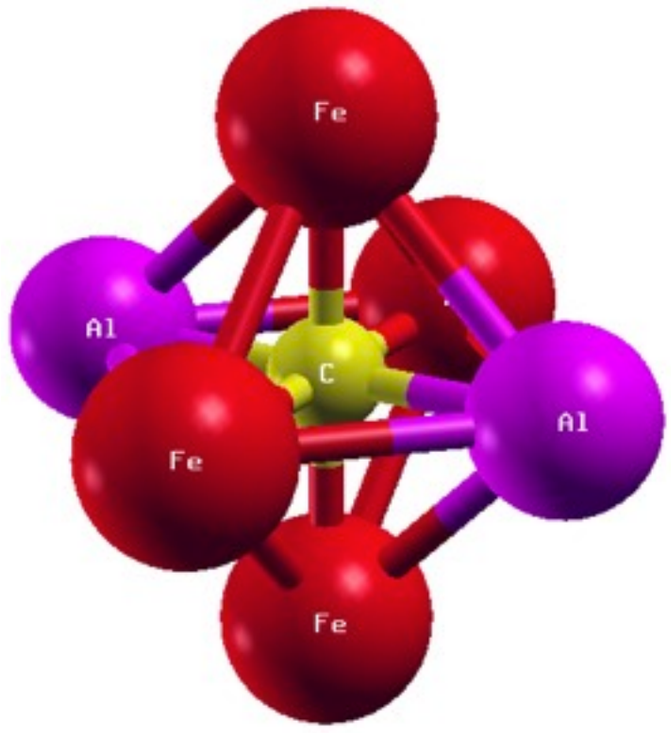


Figure 11. Bar diagram showing the specific energy absorption $E^{V}_{spec.}$ of a TRIPLEX steel and a TWIP steel in comparison to conventional deep drawing steels at the crash relevant strain rate of $\dot{\varepsilon} = 10^2\ s^{-1}$.

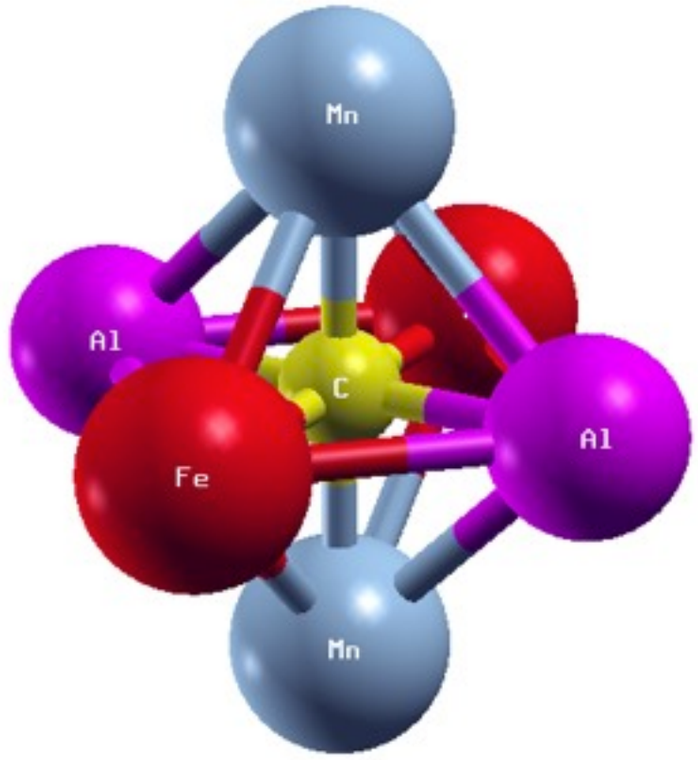
G. Frommeyer and U. Brux, 2006, steel research int. **77** (2006)



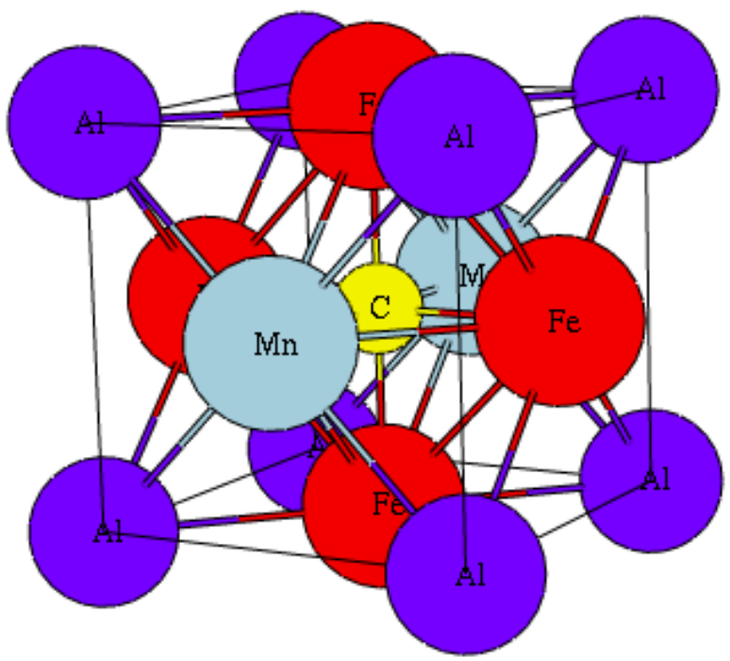
κ-carbide (octa. 1)

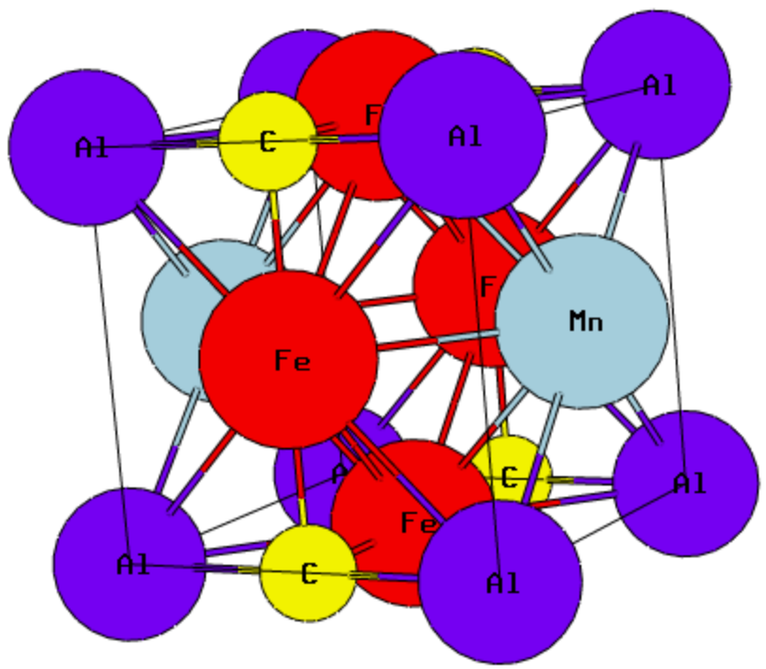


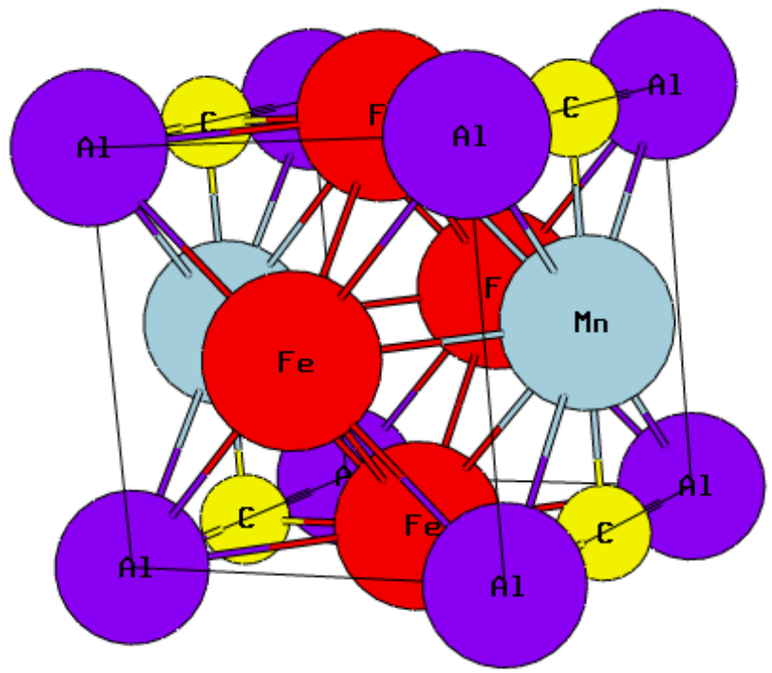
Octa. 2



Octa. 3







Main problem

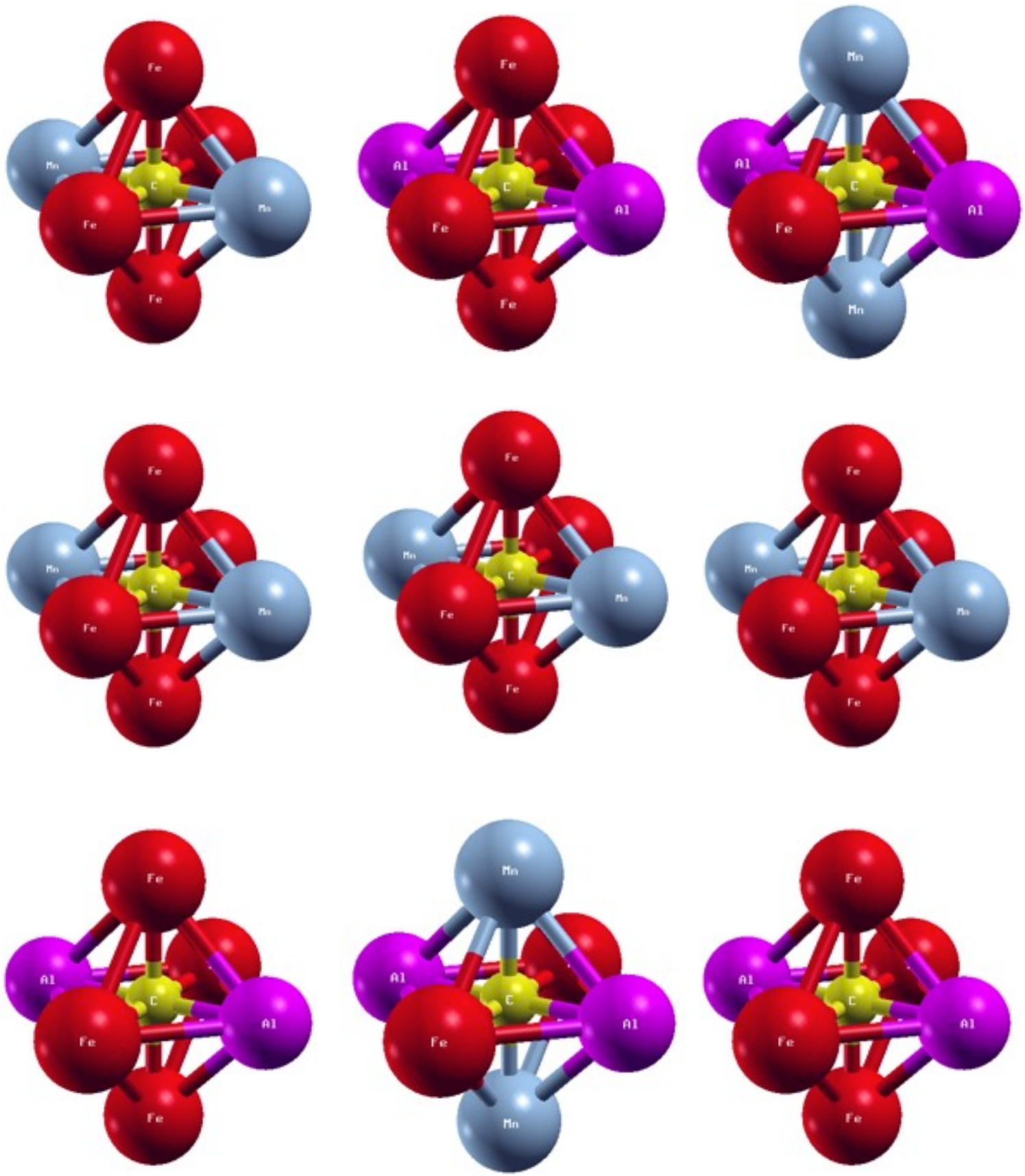
Compounds	CALPHAD assessment	FLAPW*	Pseudo Potential*
$L1_2$ Fe_3Al	-17.5[a], -19.3[b]	-8.8[c]	-19.3[d], -21.4[e]
$E2_1$ Fe_3AlC	-18.2[a], -16.0[b]	-27.9[c]	-18.4[e]
$E2_1$ Mn_3AlC	-27.3[a]	-	-

in kJ/atom − mol

Reassess the ab initio result to finite temperature.

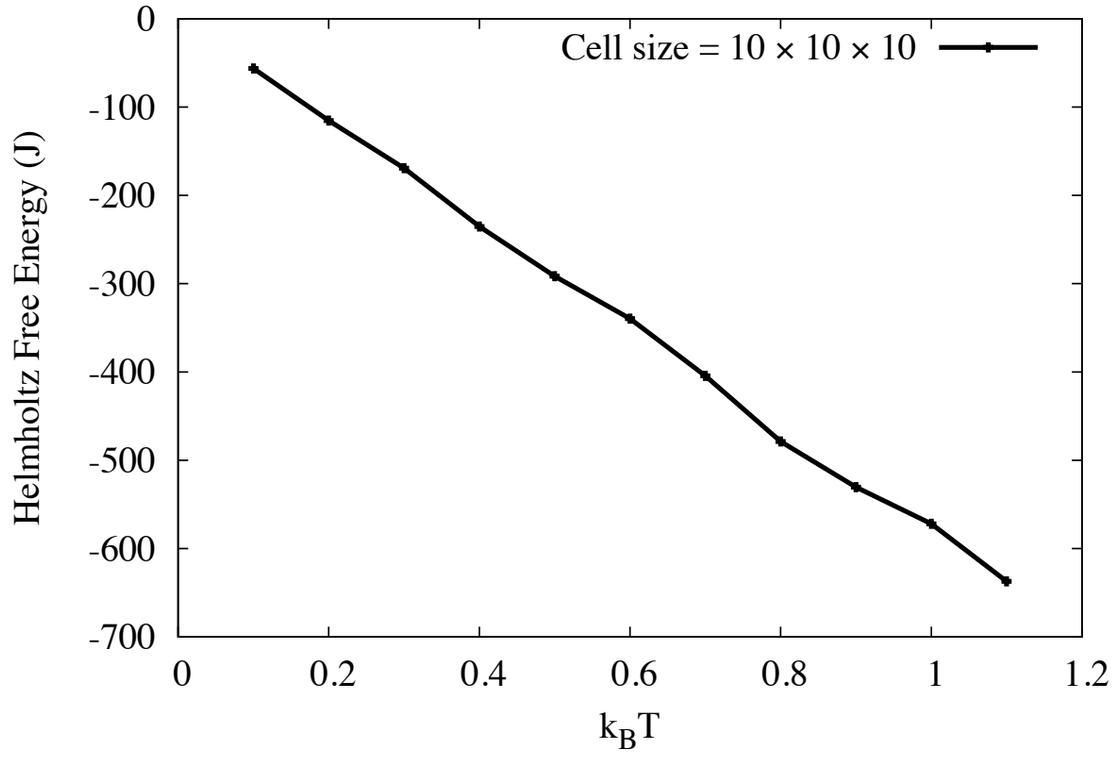
Determine physical properties :
bulk modulus, elastic constant, etc.

Monte-Carlo simulation



Monte-Carlo results

- There is no phase transition.
- C++ can't deal a number over 10^{256}.
- If once the variable (for example, DOS) became bigger than limit, log value is also goes to infinite.
- ∴ we should separate bottom and exponent.



$F_{Helmholtz} = kT \ln(\text{sum of DOS})$

Thank you!