



# Module #26

## Ordered Alloys

### READING LIST

1. Chapter 12, Meyers & Chawla.
2. Y. Umakshi, "Deformation of Intermetallic Compounds," in Materials Science and Technology: A Comprehensive Treatment, Vol. 6, Plastic Deformation and Fracture of Materials, R.W. Cahn, P. Haasen and E.J. Kramer editors, (VCH Publishers, New York, 1993) Ch. 6, pp.251-310
3. Various handouts

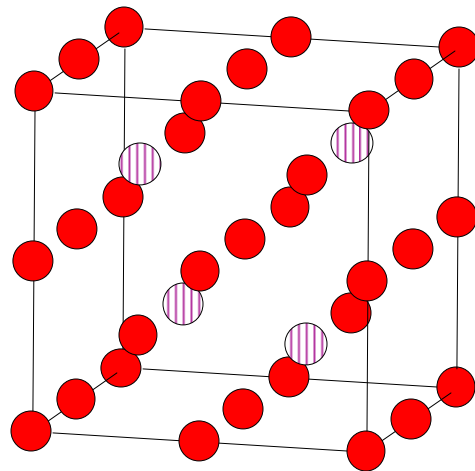


# What is an intermetallic?

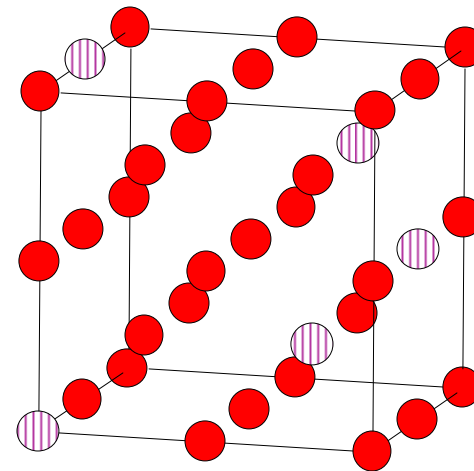
- An intermetallic is *a compound phase consisting of two or more metallic elements*. Intermetallic compounds can be *ordered* or *disordered*.
- There are some 300 intermetallic compounds with melting temperatures above 1,500°C. For this reason there is great interest in developing intermetallic-based alloys and composites for elevated temperature applications.
- Intermetallics also exhibit a number of other attractive properties:
  - Many are very resistant to oxidation and corrosion.
  - Most have very low densities relative to conventional structural materials.
  - Many form strongly adherent surface oxide films.
  - Some exhibit unique optical and magnetic properties (e.g., ordered NiPd and NiPt alloys).
  - Etc.

# Ordered intermetallics

- In ordered intermetallics, atoms assume specific atomic sites within the lattice.



Ordered



Disordered

- The strong bonding that is observed in ordered structures imparts them with:
  - Complex dislocations in comparison to disordered alloys
  - Unusual mechanical behavior (because dislocations are different)
  - Differences in other properties as well.

# Properties of some common intermetallics

Compound	Structure	Melting Point, °C	Density, g/cc	Elastic Modulus, GPa
FeAl	B2 "Ordered bcc"	1250-1400	5.6	263
Fe <sub>3</sub> Al	DO <sub>3</sub>	1540	6.7	---
Ni <sub>3</sub> Al	L1 <sub>2</sub> "Ordered fcc"	1390	7.5	337
TiAl	L1 <sub>0</sub> "Ordered tetragonal"	1460	3.9	94
Ti <sub>3</sub> Al	DO <sub>19</sub> "Ordered hcp"	1600	4.2	210
MoSi <sub>2</sub>	Tetragonal	2020	6.31	430
NiAl	B2 "Ordered bcc"	1640	5.9	206
Fe	bcc	1538	7.9	211
Ni	fcc	1455	8.9	200
Ti	hcp	1669	4.5	116

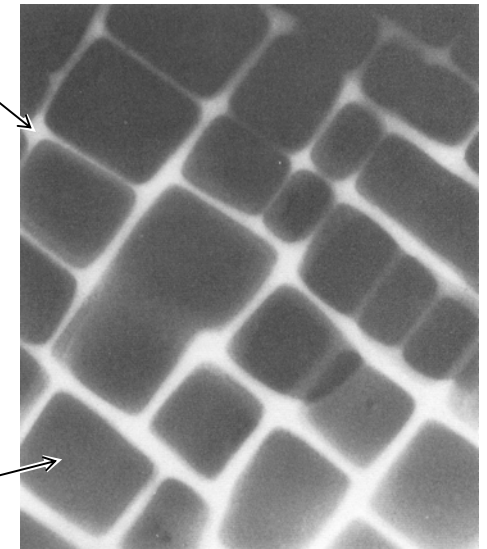
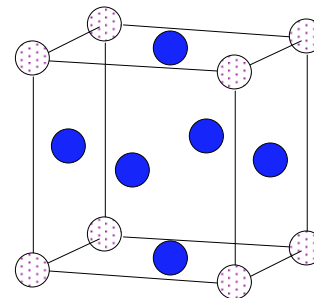
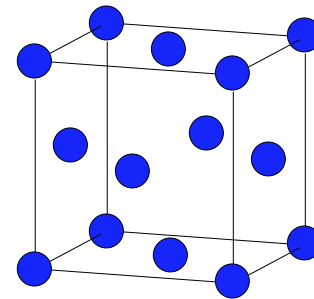
# Ni-base superalloys

- Intermetallic precipitates are the primary reason that they are so strong.

- Phases:

- Ni solid solution ( $\gamma$  – gamma)

- $\text{Ni}_3\text{Al}$  ( $\gamma'$  – gamma prime) precipitates get stronger as temperature increases. This is an intermetallic.



ASM Specialty Handbook on Heat Resistant Materials, p. 266

Cube-on-cube OR  
 $\{100\}\gamma // \{100\}\gamma'$   
 $\langle 100 \rangle\gamma // \langle 100 \rangle\gamma'$

Why does this occur in  $\gamma'$  when  $\gamma$  gets weaker as T increases?

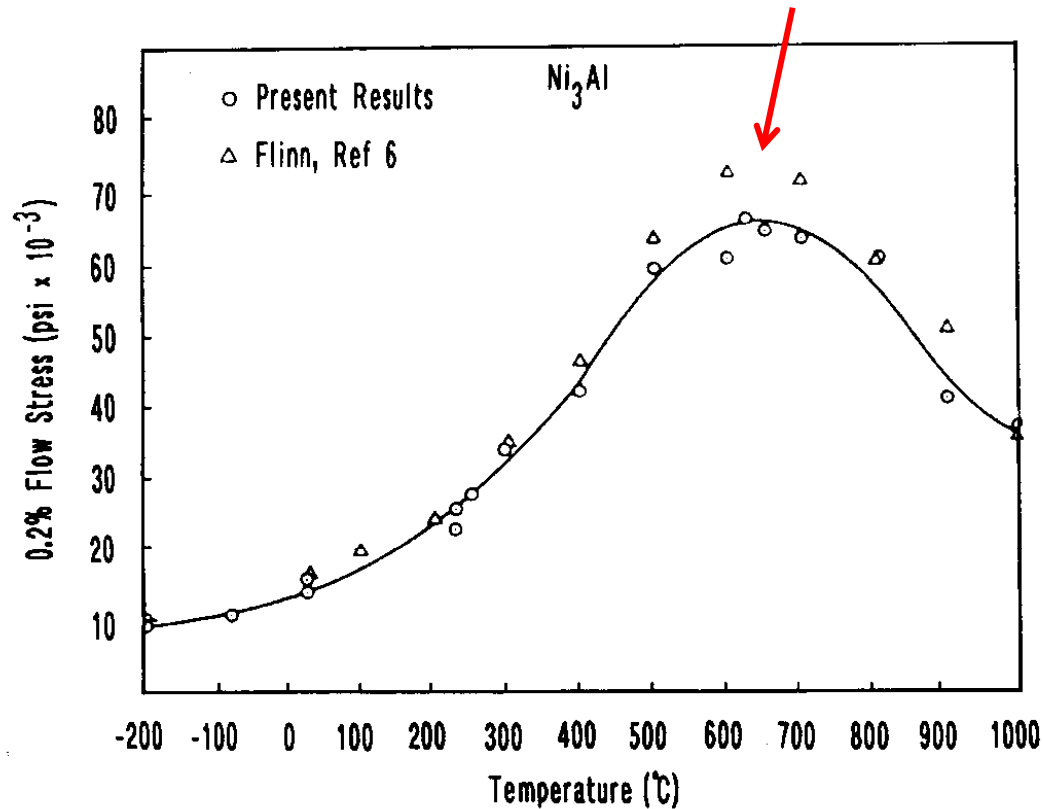
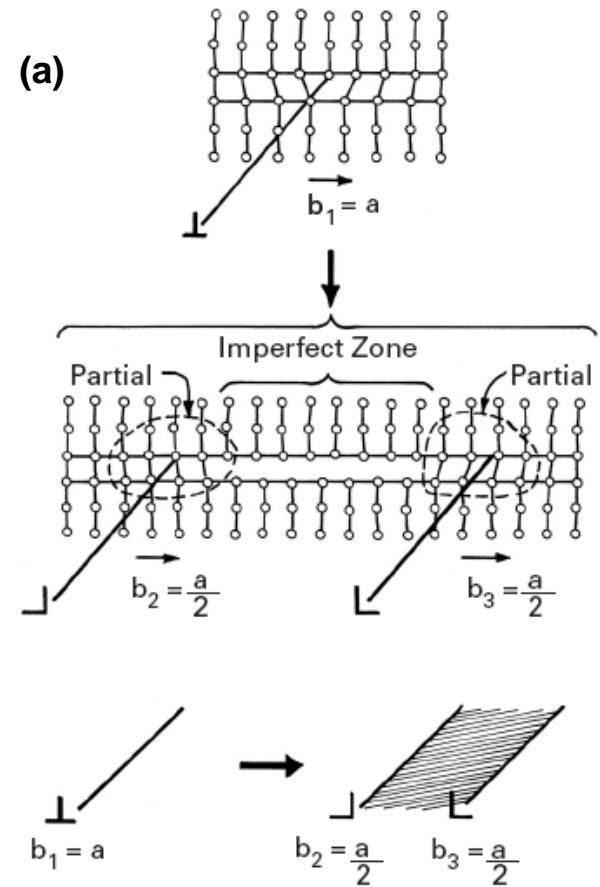


Figure 5.6. Temperature dependence of the proportional limit of alloys of the type  $Ni_3Al$ , after Davies and Stoloff (1965a): circles – Davies and Stoloff (1965),  $Ni_{86}Al_{14}$ ; triangles – Flinn (1960),  $Ni_{70}Al_{20}Fe_{10}$ ; reprinted with permission from Transactions of The Metallurgical Society of AIME, **218**, p. 714, Flinn 1960 and **233**, p. 145, 1965, a publication of The Minerals, Metals and Materials Society, Warrendale, Pennsylvania 15086.

Nabarro and de Villiers, *Physics of Creep*,  
Taylor Francis, London (1995) p. 109.

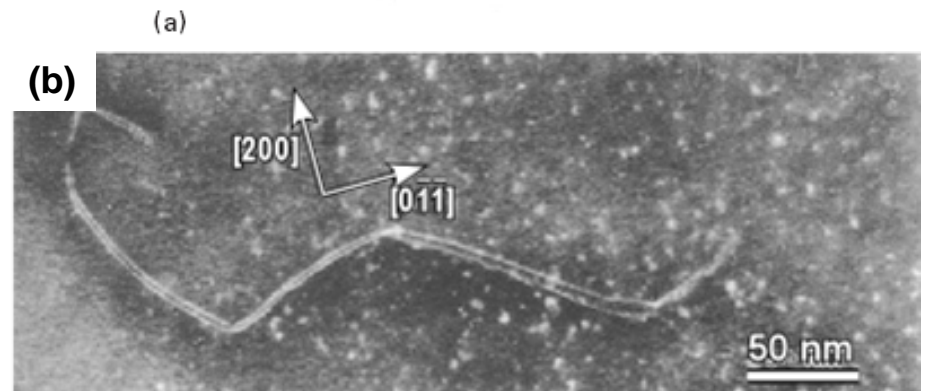
# Dislocation structures in ordered intermetallics

- Dislocation structures in ordered alloys consist of two superpartial dislocations separated by an antiphase boundary (APB).
- DO YOU RECALL WHY?**
- The whole thing is illustrated for  $\text{Ni}_3\text{Al}$  on the right.



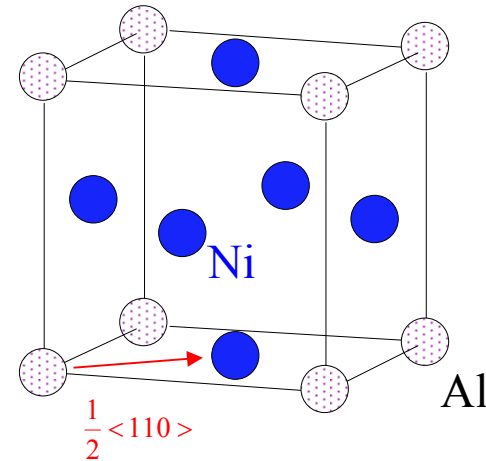
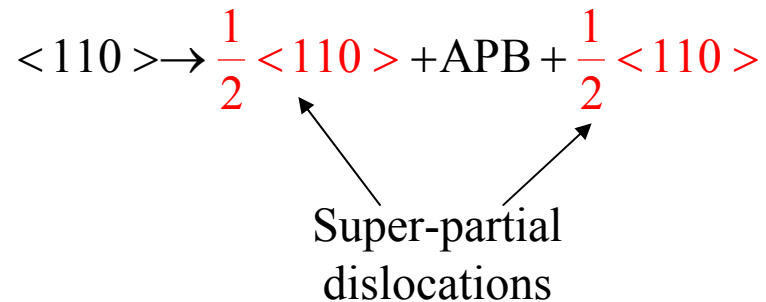
## Figure

(a) The characteristic dislocation structure in an ordered. (b) Superpartial dislocations separated by  $\sim 5$  nm in  $\text{Ni}_3\text{Al}$  deformed at  $800^\circ\text{C}$ .  $\mathbf{b} = [110]$  and superpartials  $\mathbf{b}_1 = \mathbf{b}_2 = \frac{1}{2} [110]$ . [Figure Adapted from Meyers & Chawla, 2<sup>nd</sup> edition, p. 625.]



# Super-dislocations

$L1_2$  dislocations



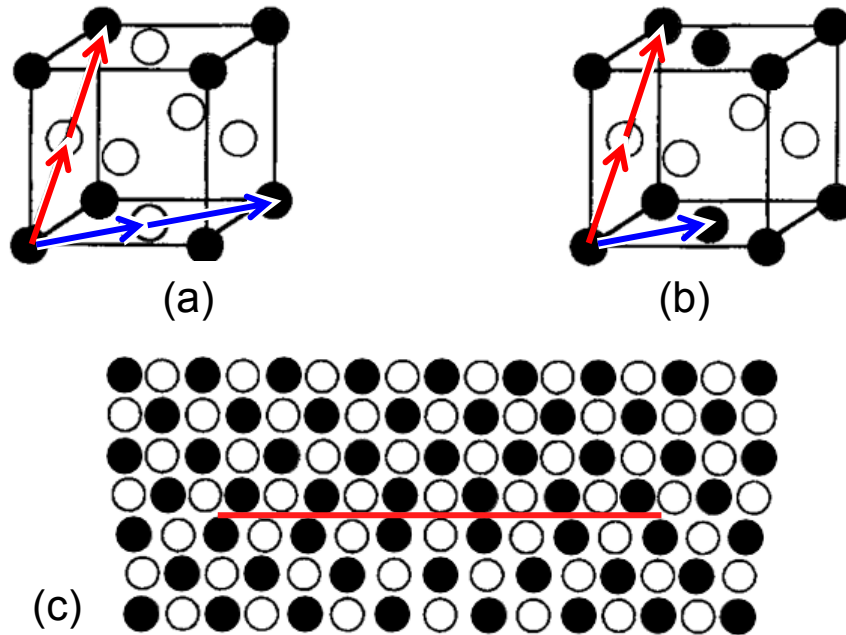
APB = anti-phase boundary

a chemical fault in which a preferred atom is not in the right chemical position.

2 shears are required to put the atoms back in their correct chemical positions.



## superdislocations



**Figure 9.38** Ordered structures and antiphase boundaries (APB): (a) the ordered, FCC-related  $L1_2$  unit cell; (b) the ordered FCC-related  $L1_0$  unit cell; (c) an AB in an idealized ordered cubic lattice (embodied by the red horizontal line). Along the APB plane, like atoms are located in nearest-neighbor positions. The APB is bordered by two partials that would be perfect dislocations if the lattice were disordered. [Image adapted from, P. Veysseyre, “Dislocations and the Plasticity of Crystals”, in Mechanics and Materials: Fundamentals and Linkages, M.A. Meyers et al. editors, (Wiley, New York, 1999) Ch. 9, p. 343]

- The passage of two partial dislocations and an APB is termed a **superdislocation** (or **superlattice dislocation**). WHY? It has a Burgers vector that is twice as large as that of the parent disordered structure.

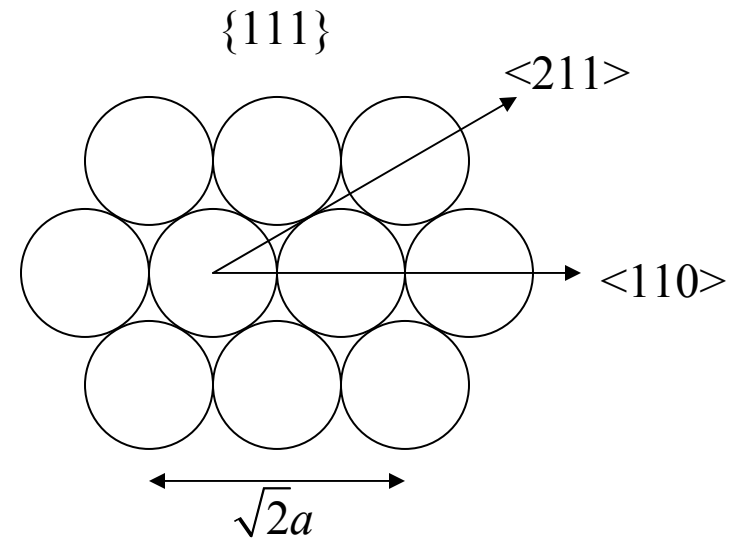
$$b \rightarrow \underbrace{\frac{b}{2} + APB + \frac{b}{2}}_{\text{Superdislocation}} = \text{partial } \perp + APB + \text{partial } \perp$$

# Strengthening in ordered phases

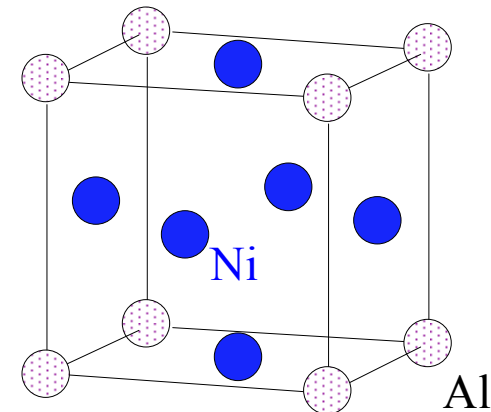
- Common FCC dislocations

$$\frac{1}{2} \langle 110 \rangle \rightarrow \frac{1}{6} \langle 211 \rangle + \text{ISF} + \frac{1}{6} \langle 1\bar{2}1 \rangle$$

Refresher: Why  $\{111\}$  planes?  
 Why are they  $\frac{1}{2}\langle 110 \rangle$  dislocations?  
 Why are they  $\frac{1}{6}\langle 211 \rangle$  types?



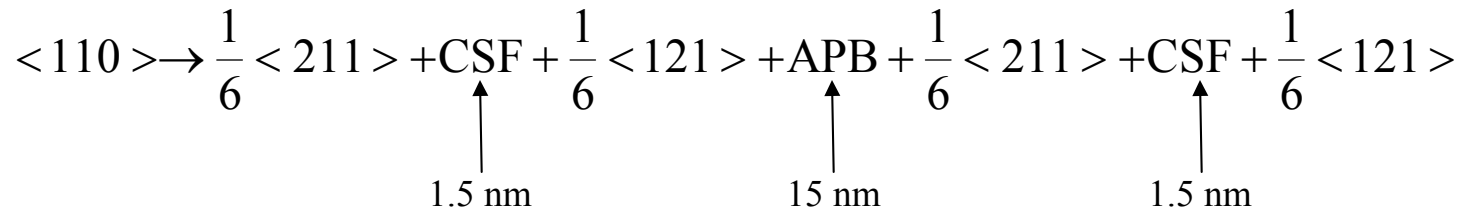
- Since  $L1_2$  is an ordered phase, the full dislocation is  $[110]$  and its partials are  $\frac{1}{2}[110]$ .
  - Passing a single dislocation through  $\gamma'$  would generate an APB and increase energy.



ISF = intrinsic stacking fault

# Super-partial dislocations

- Superpartial dislocations can dissociate into a pair of Shockley-like partials.
- An intrinsic (unoccupied stacking site) and chemical stacking fault forms (change in chemical environment about sheared atom) → complex stacking fault (CSF)



Stacking Fault = occupying an unoccupied site in the normal stacking sequence

APB = *not a stacking fault*, occupying a normal stacking site but not the correct chemical stacking site.

CSF = a combination of stacking fault and APB

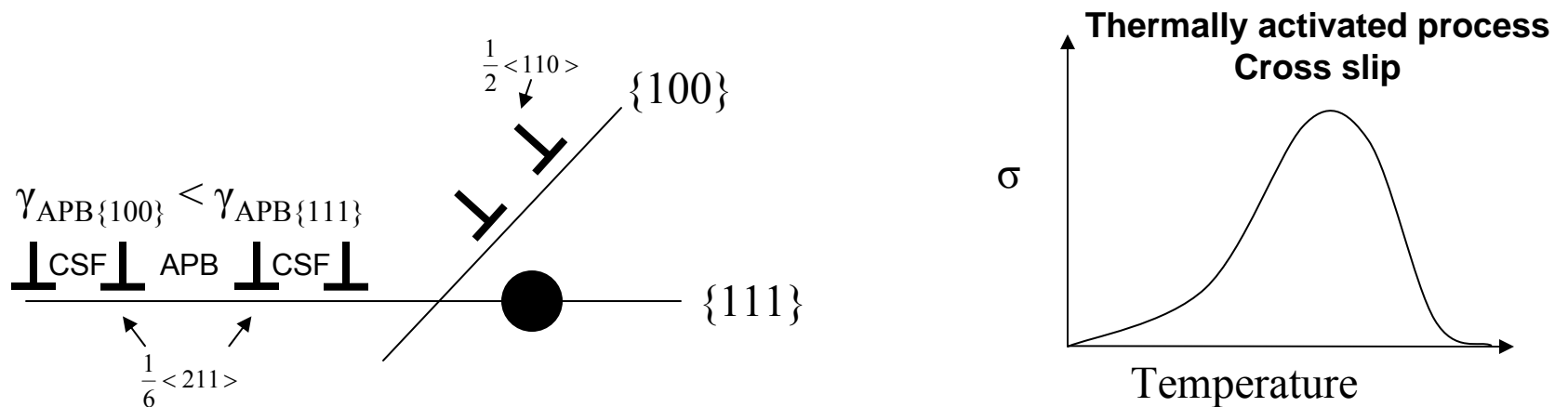
# Kear-Wilksdorf locks

Why do dislocations separate into partials? What keeps the partials together?

Dislocations on  $\{111\}$  planes **cross slip** on cube plane. Why?

Dislocations on cube plane become locked (high Peierls stress on  $\{001\}$ ) and do not propagate.

More and more dislocations cross slip and become locked. This increases the hardness at elevated temperatures until the thermal energy becomes sufficient to overcome the Peierls stress and glide.



# Cross-slip continued

- If dislocations are locked on cube plane, why don't they cross slip back onto  $\{111\}$ ?
- Explained by Paider, Pope & Vitek (PPV) model.
  - Dislocation core is spread and not contained in all of the plane.
  - When cross slipped, core not in the plane, dislocation locks (core off the cube plane).
  - Temperature increases  $\rightarrow$  core constricted, constricts the partials  $\rightarrow$  cross slip back on  $\{111\}$ .



















# Dislocation structures in ordered intermetallics

- In ordered alloys such as Ni<sub>3</sub>Al, FeAl, TiAl, etc., movement of dislocations and vacancies results in destruction of the local order, which yields a higher energy state.
- A second dislocation must pass through the lattice to restore order and reduce the energy state to a minimum.
- This requirement places restrictions on dislocation motion and upon the motion of vacancies.
- It is quite complicated.

## Restricted dislocation motion

- Such defect structures are restricted because motion of the APB is dictated by cross-slip of the partial dislocations bounding the APB.
- This becomes even more complicated in ordered fcc structures like the ones illustrated on the previous page because the partial dislocations can break down into even smaller segments resulting in *superpartials* on either side of the APB.
- The table on the following viewgraph illustrates some possible dislocation morphologies for some interesting ordered alloys.

## Dislocation morphologies for some ordered alloys

Superlattice type	Chemical designation	Unit Cell Dimensions	Alloy Types	Superlattice Dislocation Type	Burgers Vector of each Dislocation	Antiphase Boundary Type
B2	CsCl	$a_o$	NiAl, AgMg AuZn	$\perp$	$a_o \langle 100 \rangle$	none
			CuZn, FeCo FeAl, FeRh NiAl, AgMg AuZn		$\frac{a_o}{2} \langle 111 \rangle$	 NN
DO <sub>3</sub>	Fe <sub>3</sub> Al	$a_o$	Fe <sub>3</sub> Al, Fe <sub>3</sub> Si Fe <sub>3</sub> B		$\frac{a_o}{4} \langle 111 \rangle$	 NN  NNN
L1 <sub>2</sub>	Cu <sub>3</sub> Au	$a_o$	Cu <sub>3</sub> Au, Ni <sub>3</sub> Mn Ni <sub>3</sub> Al, Ni <sub>3</sub> Fe Cu <sub>3</sub> Pd, Ni <sub>3</sub> Ti Ag <sub>3</sub> Mg, Ni <sub>3</sub> Ta Ni <sub>3</sub> Ga		$\frac{a_o}{6} \langle 112 \rangle$	 NN  NN + SF
DO <sub>19</sub>	Mg <sub>3</sub> Cd	$a_o$ $c_o$	Mg <sub>3</sub> Cd, Ti <sub>3</sub> Al		$\frac{a_o}{6} \langle 10\bar{1}0 \rangle$	 NN
					$\frac{a_o}{2} \langle 2\bar{1}\bar{1}0 \rangle$	 SF  NNN
L1 <sub>0</sub>	CuAu	$a_o$ $c_o$	CuAu, CoPt FePt, TiAl		$\frac{a_o}{6} \langle 112 \rangle$	 NN
						 NN + SF  SF

NN = nearest neighbor ; NNN = next nearest neighbor ; SF = stacking fault

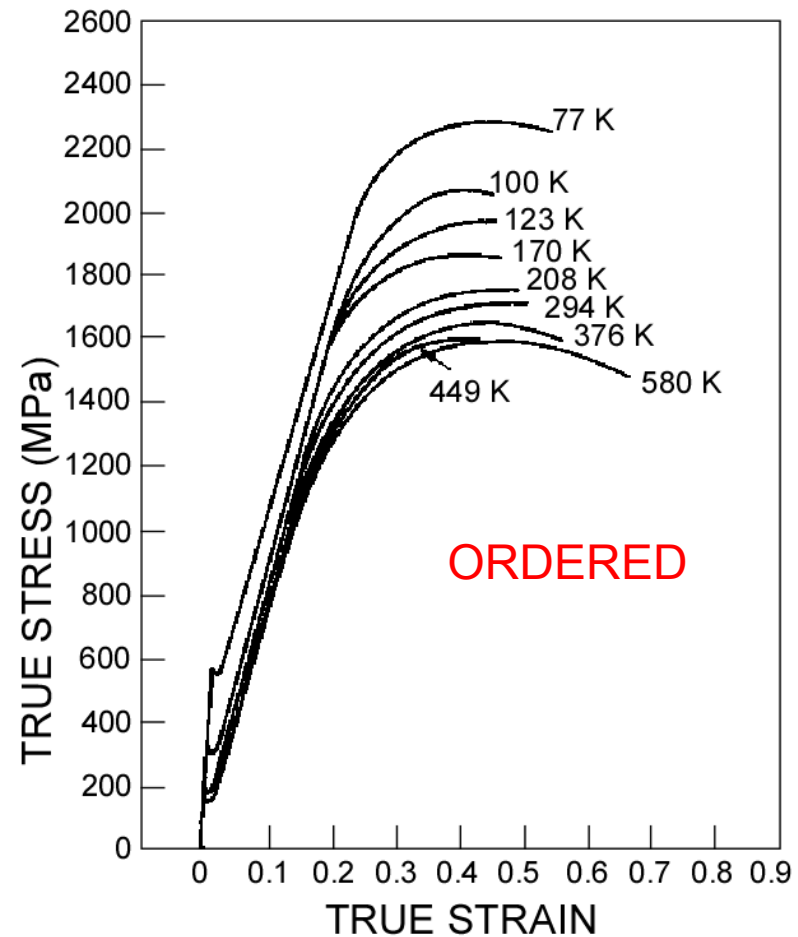
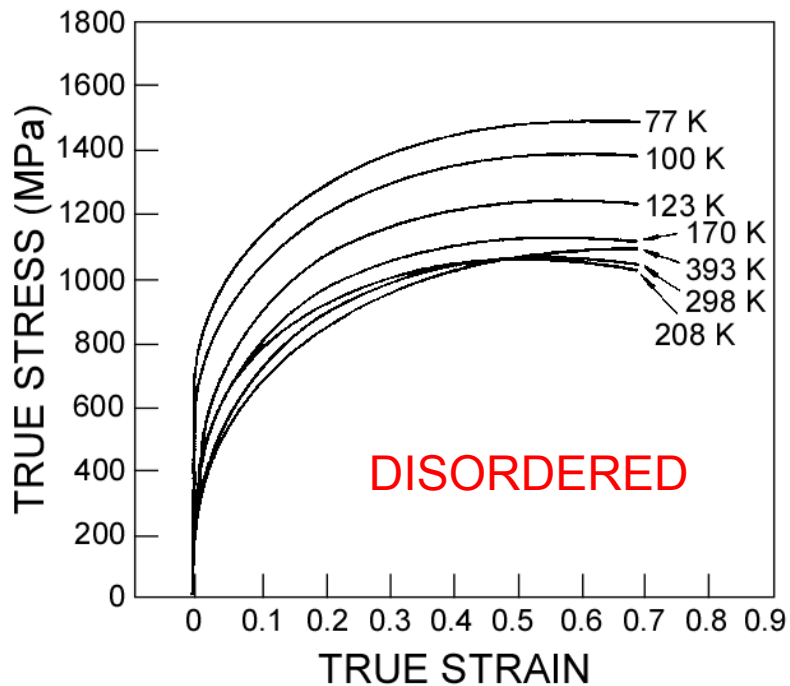
$$b \rightarrow \underbrace{\frac{b}{2} + APB + \frac{b}{2}}_{\text{Superdislocation}} = \text{partial } \perp + APB + \text{partial } \perp$$

Table adapted with corrections from Meyers & Chawla, 1<sup>st</sup> Edition, p. 530. Originally from M.J. Marcinkowski, Treatise on Materials Science and Technology, V. 5 (New York, Academic Press, 1976, p. 181).



# Implications of order

- ordered alloys exhibit significantly higher yield and flow stresses.



Stress-strain curves for fully disordered and ordered FeCo. [Adapted from S.T. Fong, K. Sadananada, and M.J. Marcinkowski, *Metall. Trans.* **5** (1974) 1239-1247]

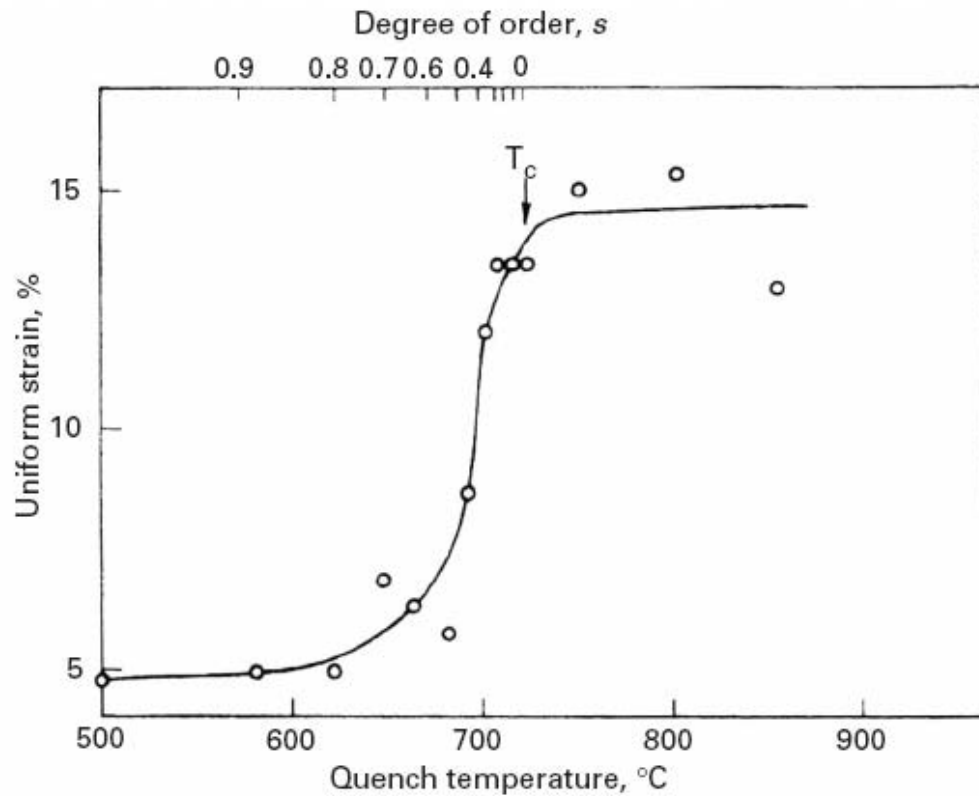
## Implications of order

- Fully ordered alloys deform by means of the movement of **superlattice dislocations** at low stresses.
- Superdislocations must move as a group to maintain the ordered crystal structure.
- This **restricts cross-slip** which leads to higher strain hardening rates and higher strengths than are observed in disordered materials.

# How does ordering influence:

- Fatigue resistance?
- Precipitation hardened alloys?
- Creep strength?

# Effect of Ordering on Ductility

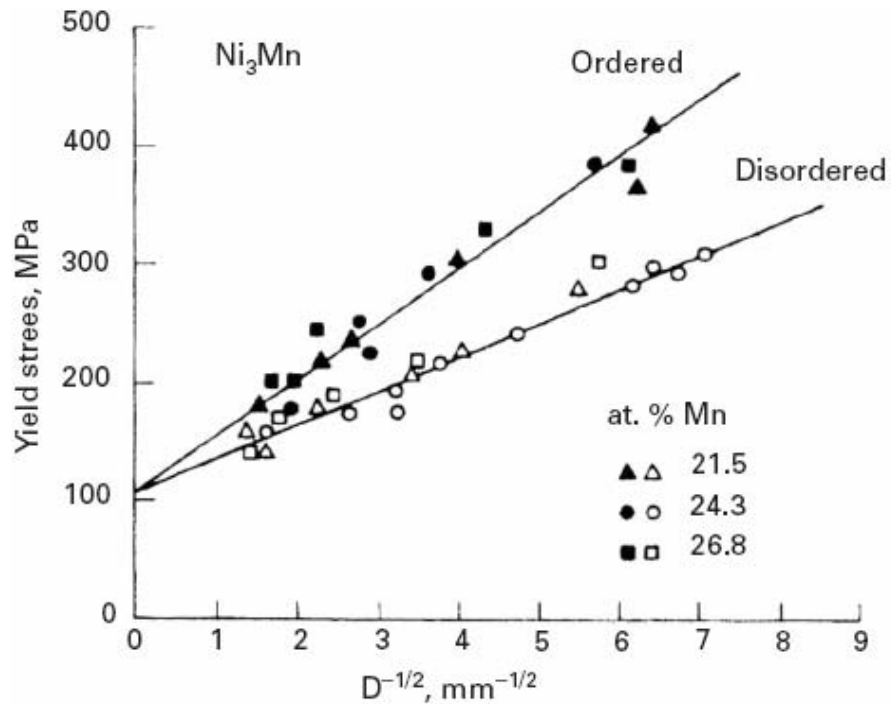


Effect of atomic order on uniform strain (ductility) of Fe-Co-2% V at 25 °C.

Meyers & Chawla, 2<sup>nd</sup> Ed., p. 630.

(Adapted with permission from N. S. Stoloff and R. G. Davies, *Acta Met.*, 12 (1964) 473.)

# Hall-Petch Relationship

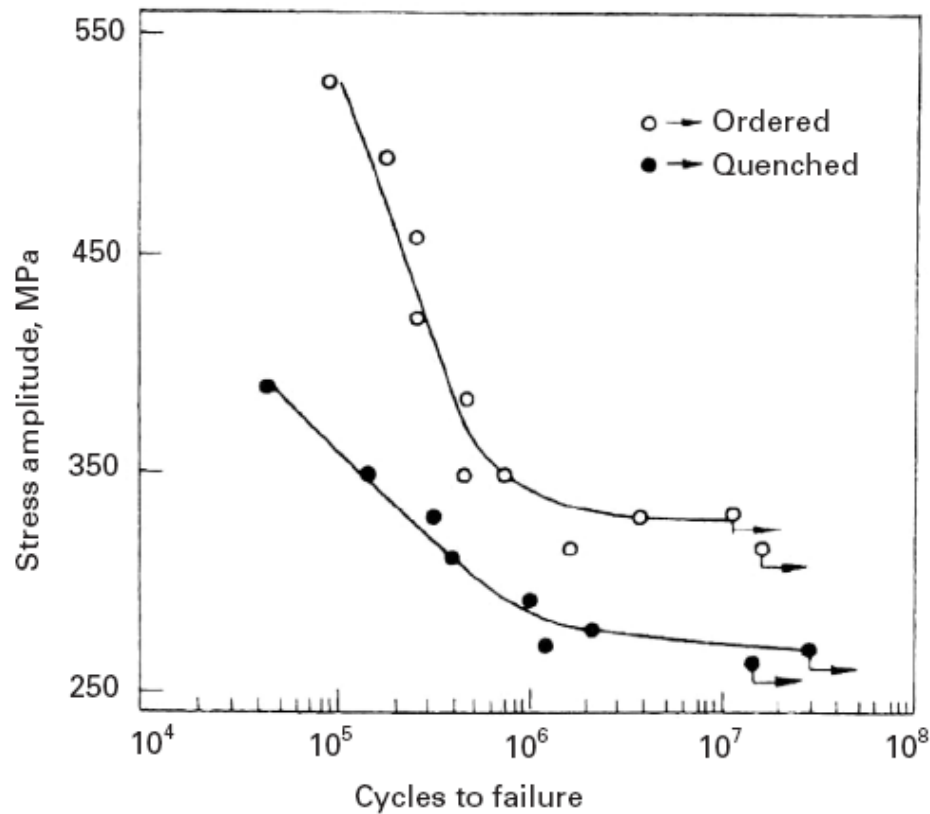


Hall–Petch relationship for ordered and disordered alloys.

Meyers & Chawla, 2<sup>nd</sup> Ed., p. 630.

(Adapted with permission from T. L. Johnston, R. G. Davies, and N. S. Stoloff, *Phil Mag.*, 12 (1965) 305.)

# Fatigue Behavior

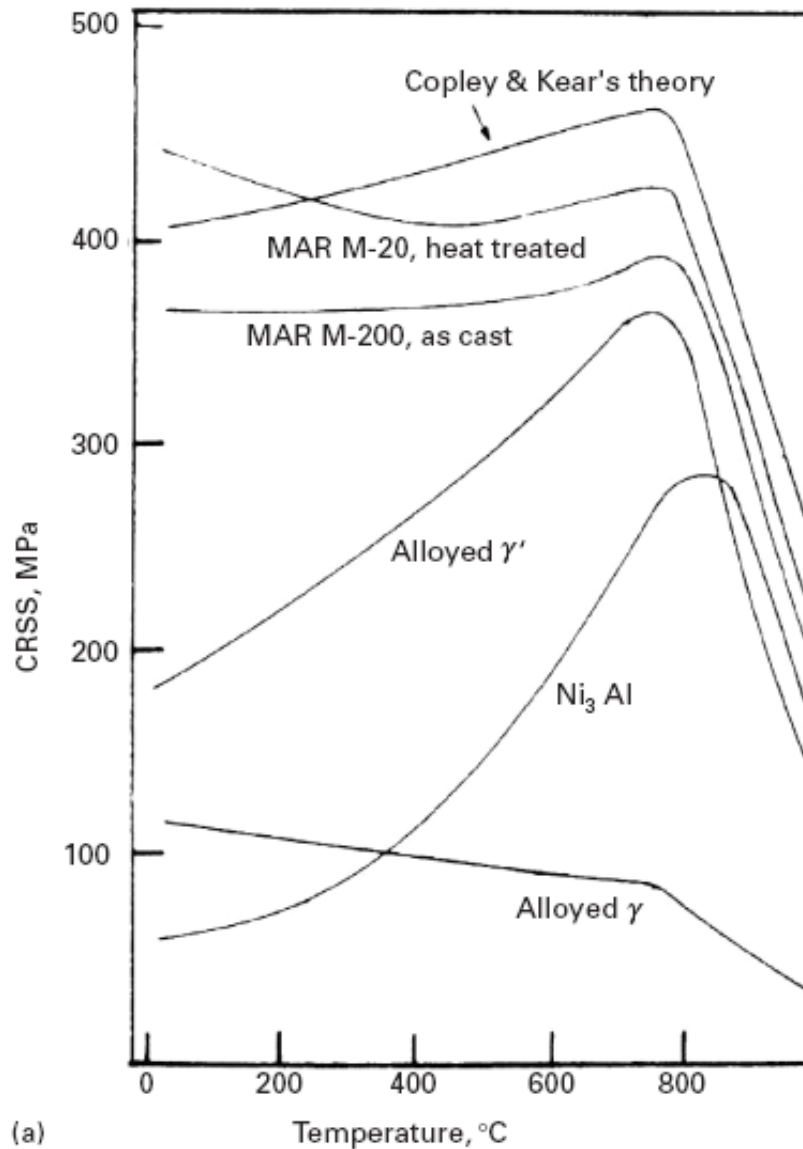


Effect of atomic order on fatigue behavior of Ni<sub>3</sub>Mn.

Meyers & Chawla, 2nd Ed., p. 631.

(Adapted with permission from R. C. Boettner, N. S. Stoloff, and R. G. Davies, *Trans. AIME*, 236 (1968) 131.)

# Strengthening in $\text{Ni}_3\text{Al}$ , $\gamma$ , and Mar M-200

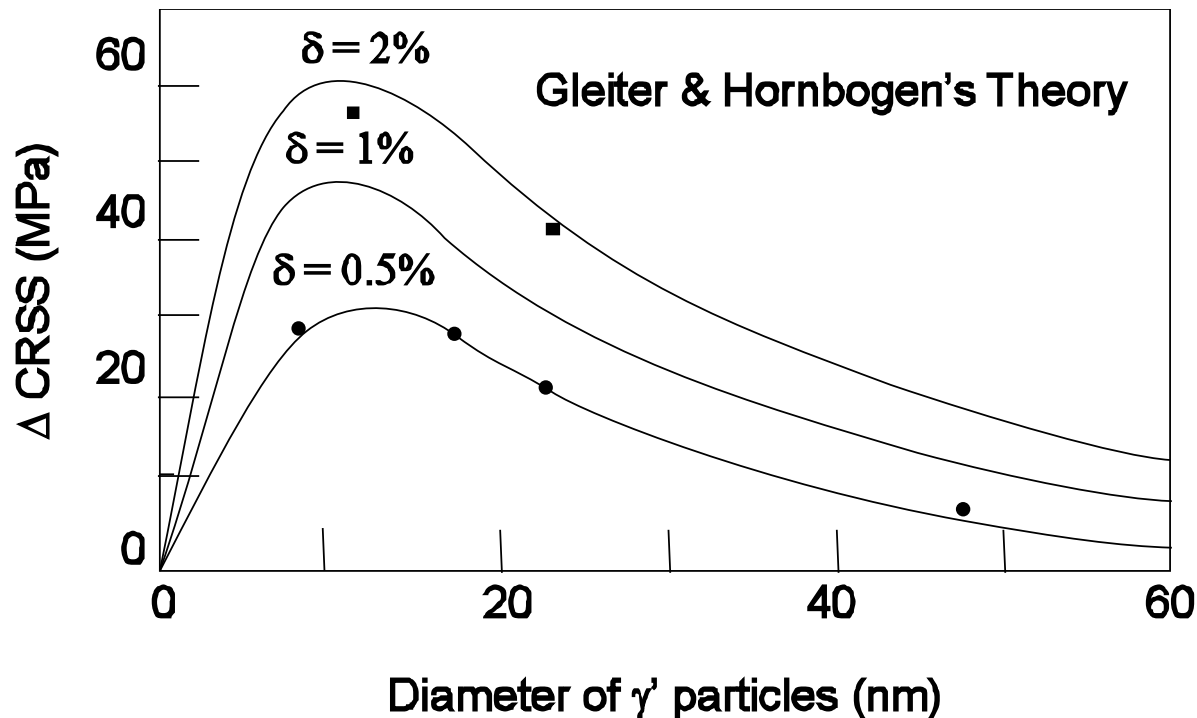


(a) Effect of temperature on CRSS for  $\text{Ni}_3\text{Al}$ ,  $\gamma$ , and Mar M-200 superalloy ( $\gamma + \gamma'$ ).

Meyers & Chawla, 2<sup>nd</sup> Ed., p. 632.

(Adapted with permission from S. M. Copley and B. H. Kear, *Trans. TMS-AIME*, 239 (1967) 987.)

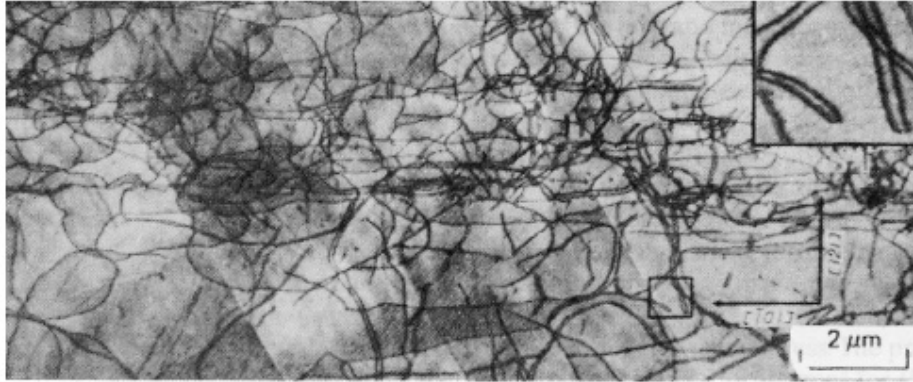
# Precipitation Hardening



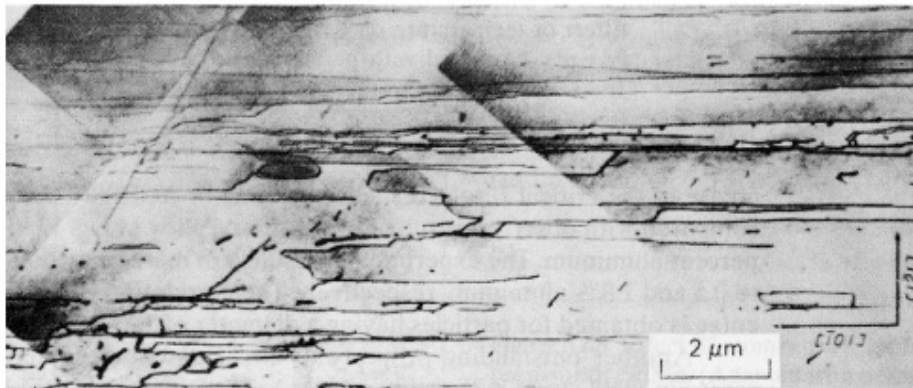
Calculated and observed increase in the critical resolved shear stress (CRSS) in a Ni–Cr–Al alloy as a function of the diameter of the precipitate; full lines represent calculations;  $\delta$  is atomic percent aluminum. [From Meyers & Chawla, 2<sup>nd</sup> Ed., p. 632 (Adapted with permission from H. Gleiter and H. Hornbogen, *Phys. Status Solids*, 12 (1965) 235.)]



# Effect of Temperature on Dislocation Configuration



(a)



(b)

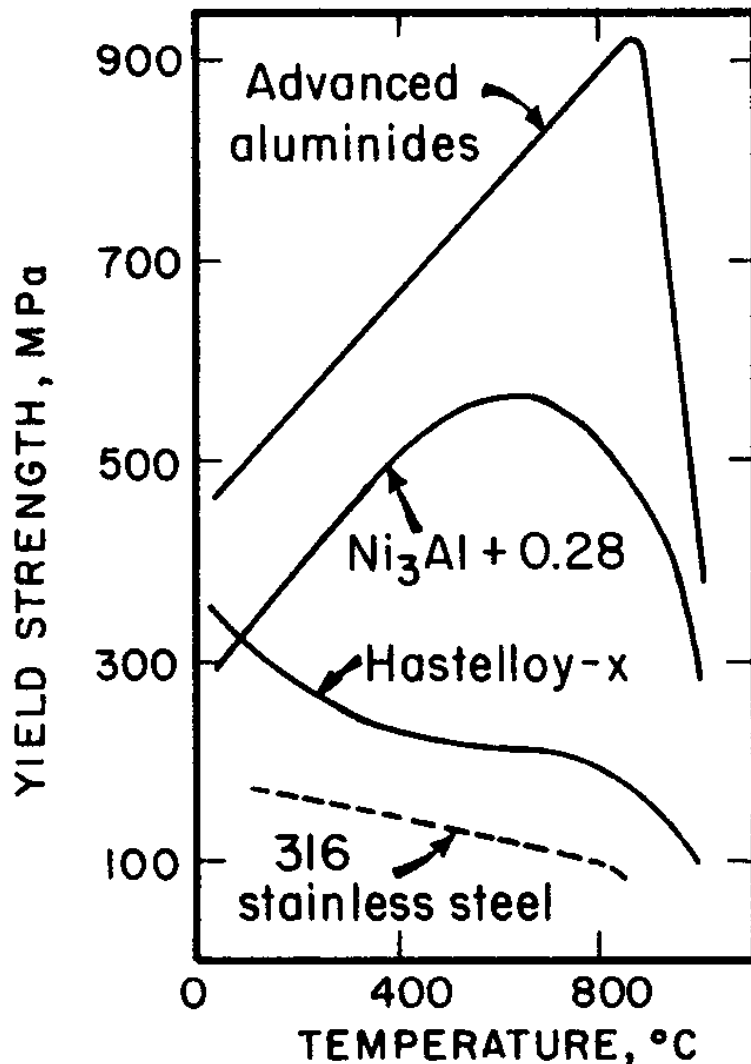
Effect of deformation temperature on the dislocation arrangement in the  $\{111\}$  primary slip plane of ordered  $\text{Ni}_3\text{Ge}$ .

(a)  $T = -196 \text{ }^\circ\text{C}$ ,  $\varepsilon_p = 2.4\%$ .

(b)  $T = 27 \text{ }^\circ\text{C}$ ,  $\varepsilon_p = 1.8\%$ .

Meyers & Chawla, 2<sup>nd</sup> Ed.,  
p. 633.

# Effect of Temperature on Strengthening



Yield stress as a function of test temperature for Ni<sub>3</sub>Al based aluminides, Hastelloy-X, and type 316 stainless steel.

(Adapted from C. T. Liu and J. O. Stiegler, *Science*, 226 (1984) 636.)