

# 23. Crystal Physics

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Jan. 10, 2018

# Nonlinear optics

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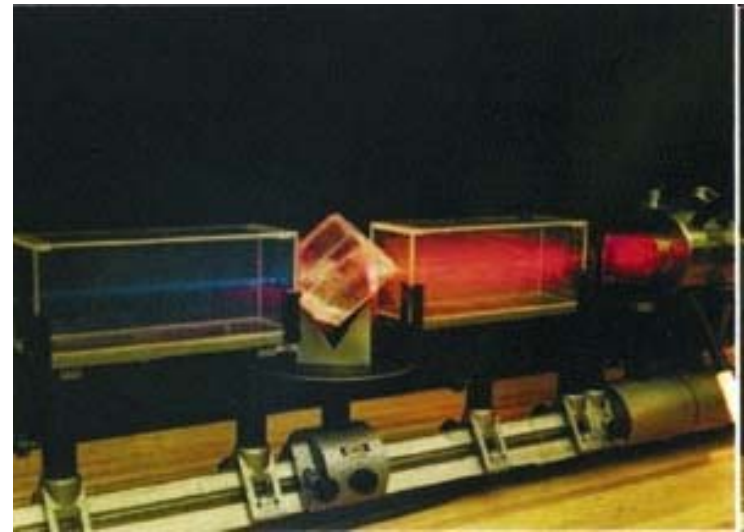
Period doubling crystals

no inversion symmetry

$$P = \chi^{(1)} E + \chi^{(2)} E^2 + \chi^{(3)} E^3 + \dots$$

$$P_i = \frac{-\partial^2 G}{\partial E_i \partial E_j} E_j + \frac{1}{2} \frac{-\partial^3 G}{\partial E_i \partial E_j \partial E_k} E_j E_k + \dots$$

$$\cos^2(\omega t) = \frac{1}{2}(1 + \cos(2\omega t))$$



806 nm light : lithium iodate ( $\text{LiIO}_3$ )

860 nm light : potassium niobate ( $\text{KNbO}_3$ )

980 nm light :  $\text{KNbO}_3$

1064 nm light : monopotassium phosphate ( $\text{KH}_2\text{PO}_4$ , KDP), lithium triborate (LBO).

1300 nm light : gallium selenide (GaSe)

1319 nm light :  $\text{KNbO}_3$ , BBO, KDP, lithium niobate ( $\text{LiNbO}_3$ ),  $\text{LiIO}_3$

# Birefringence (Doppelbrechung)

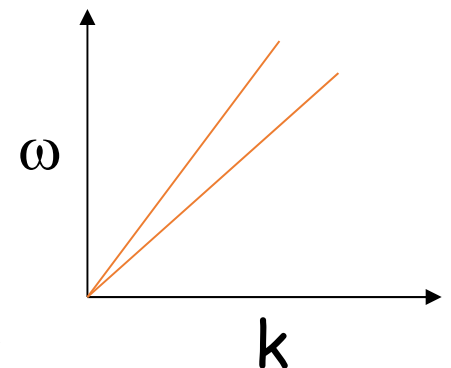
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Calcite

Two indices of refraction

<http://en.wikipedia.org/wiki/Birefringent>



# Birefringence

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## Electric susceptibility

[\[edit\]](#)

In an [isotropic](#) and [linear](#) medium, this polarisation field  $\mathbf{P}$  is proportional to and parallel to the electric field  $\mathbf{E}$ :

$$\mathbf{P} = \chi\epsilon_0\mathbf{E}$$

where  $\chi$  is the [electric susceptibility](#) of the medium. The relation between  $\mathbf{D}$  and  $\mathbf{E}$  is thus:

$$\mathbf{D} = \epsilon_0\mathbf{E} + \chi\epsilon_0\mathbf{E} = \epsilon_0(1 + \chi)\mathbf{E} = \epsilon\mathbf{E}$$

where

$$\epsilon = \epsilon_0(1 + \chi)$$

is the [dielectric constant](#) of the medium. The value  $1+\chi$  is called the *relative permittivity* of the medium, and is related to the [refractive index](#)  $n$ , for non-magnetic media, by

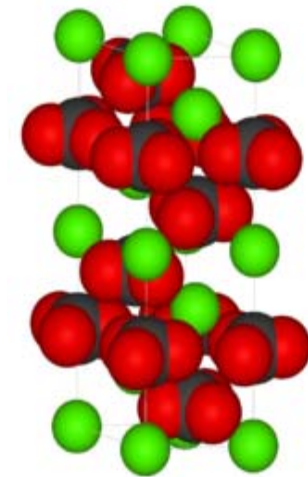
$$n = \sqrt{1 + \chi}$$

# Birefringence

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Calcite



name	international	Schoenflies	examples
rhombohedral holohedral	$\bar{3}m$	$D_{3d}$	calcite, corundum, hematite
rhombohedral hemimorphic	$3m$	$C_{3v}$	tourmaline, alunite
rhombohedral tetartohedral	$\bar{3}$	$S_6$	dolomite, ilmenite
trapezohedral	$32$	$D_3$	quartz, cinnabar
rhombohedral tetartohedral	$3$	$C_3$	none verified

# Rhombohedral crystal system

From Wikipedia, the free encyclopedia  
 (Redirected from [Trigonal crystal system](#))

In [crystallography](#), the **rhombohedral** (or **trigonal**) [crystal system](#) is one of the seven [lattice point groups](#), named after the two-dimensional [rhombus](#). A [crystal system](#) is described by three basis [vectors](#). In the rhombohedral system, the crystal is described by vectors of [equal length](#), of which all three are not mutually [orthogonal](#). The **rhombohedral system** can be thought of as the [cubic system](#) stretched [diagonally](#) along a body.  $a = b = c$ ;  $\alpha, \beta, \gamma \neq 90^\circ$ . In some classification schemes, the **rhombohedral system** is grouped into a larger [hexagonal system](#).



An example crystals, que

name	international	Schoenflies	examples
rhombohedral holohedral	$\bar{3}m$	$D_{3d}$	<a href="#">calcite</a> , <a href="#">corundum</a> , <a href="#">hematite</a>
rhombohedral hemimorphic	$3m$	$C_{3v}$	<a href="#">tourmaline</a> , <a href="#">alunite</a>
rhombohedral tetartohedral	$\bar{3}$	$S_6$	<a href="#">dolomite</a> , <a href="#">ilmenite</a>
trapezohedral	32	$D_3$	<a href="#">quartz</a> , <a href="#">cinnabar</a>
rhombohedral tetartohedral	3	$C_3$	none verified

Rhombohedral = Trigonal

<p>Trigonal  <math>\alpha, \beta, \gamma \neq 90^\circ</math></p>	$\bar{3}$	$S_6 = C_{6i}$	147-148	6
	32	$D_3$	149-155	6
	$3m$	$C_{3v}$	156-161	6
	$\bar{3}m$	$D_{3d}$	162-167	12

$$\begin{bmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{bmatrix}$$

# Optical effects

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$$P_i = P_i^0 + \frac{\partial P_i}{\partial E_j} E_j + \frac{\partial^2 P_i}{\partial E_j \partial E_k} E_j E_k + \frac{\partial^2 P_i}{\partial E_j \partial E_k \partial E_l} E_j E_k E_l + \dots$$

spontaneous  
polarization

$E_k$  DC  
Pockels effect

$E_k E_l$  DC  
Kerr effect

$$P_i = \frac{\partial^2 P_i}{\partial E_j \partial H_k} E_j H_k + \frac{\partial^2 P_i}{\partial E_j \partial H_k \partial H_l} E_j H_k H_l + \dots$$

$H_k$  DC  
Faraday effect

$H_k H_l$  DC  
Cotton–Mouton effect

**International  
Tables for  
Crystallography  
Volume D**

Physical properties of  
crystals  
Edited by A. Authier

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*International Tables for Crystallography* (2006). Vol. D, ch. 1.6, pp. 150-177  
doi: 10.1107/97809553602060000633

## Chapter 1.6. Classical linear crystal optics<sup>1</sup>

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*International Tables for Crystallography* (2006). Vol. D, ch. 1.7, pp. 178-219  
doi: 10.1107/97809553602060000634

## Chapter 1.7. Nonlinear optical properties

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# Electrostriction

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$$\frac{\partial P_k}{\partial \sigma_{ij}} = \frac{\partial \epsilon_{ij}}{\partial E_k} - \left( \frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}} \right) = d_{ijk}$$

$$\epsilon_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l + \dots$$

piezoelectricity



Electrostriction



# Rank 4 Tensors

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Stiffness tensor

Compliance tensor

Piezoconductivity

Electrostriction

Magnetostriction

How the Seebeck effect depends on stress

How the electric susceptibility depends on stress

How the magnetic susceptibility depends on stress

Nonlinear electric susceptibility

Nonlinear magnetic susceptibility

# Symmetric and asymmetric tensors

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$$-\left(\frac{\partial^2 G}{\partial E_j \partial E_k}\right) = \frac{\partial P_k}{\partial E_j} = \chi_{kj} = -\left(\frac{\partial^2 G}{\partial E_k \partial E_j}\right) = \frac{\partial P_j}{\partial E_k} = \chi_{jk}$$

## Symmetric

electric susceptibility  
magnetic susceptibility  
electrical conductivity  
thermal conductivity  
stiffness tensor

## Asymmetric

Seebeck effect  
Peltier effect  
piezoconductivity

# Anharmonic terms

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Expand the energy in terms of the normal modes of the linearized problem  $u_k$

$$U = U_0 + \frac{\partial U}{\partial u_k} u_k + \frac{1}{2} \frac{\partial^2 U}{\partial u_j \partial u_k} u_j u_k + \frac{1}{6} \frac{\partial^3 U}{\partial u_i \partial u_j \partial u_k} u_i u_j u_k + \frac{1}{24} \frac{\partial^4 U}{\partial u_h \partial u_i \partial u_j \partial u_k} u_h u_i u_j u_k + \dots$$

Thermal expansion

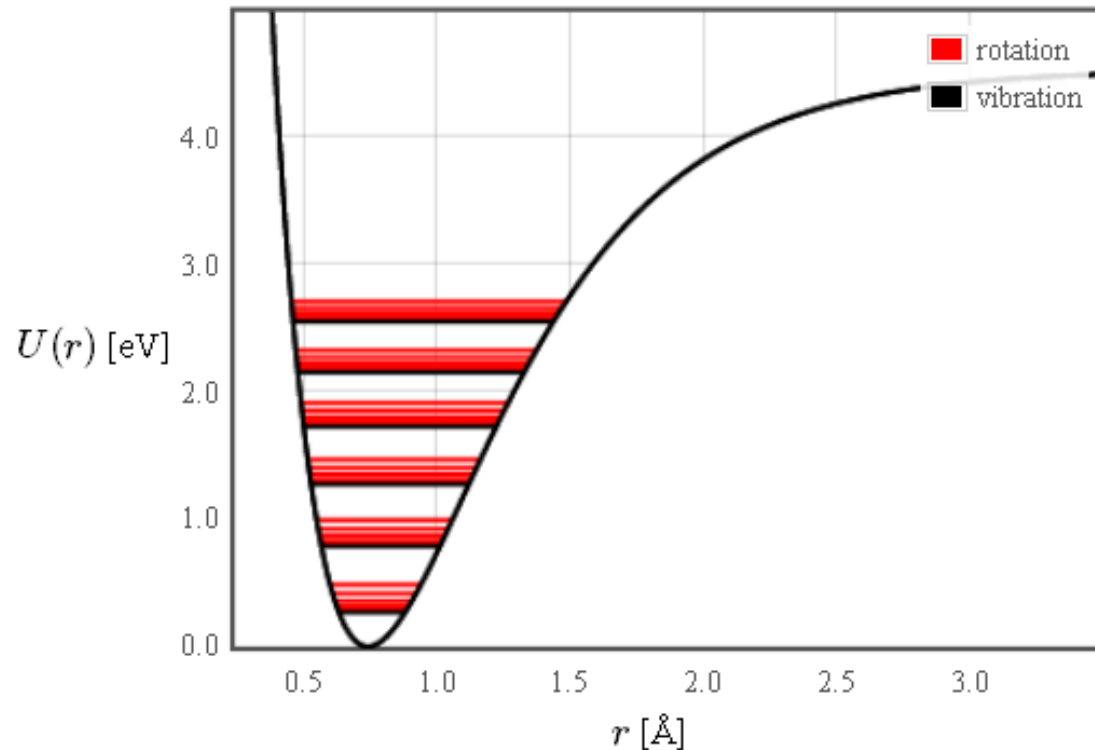
Thermal conductivity limited by Umklapp scattering

High temperature limit of specific heat does not approach the

Dulong-Petit law

# Nonlinear effects

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Thermal expansion

Thermal conductivity limited by Umklapp scattering

High temperature limit of specific heat does not approach the Dulong-Petit law

# Phase transitions

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# Structural phase transitions

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Some materials make a transition from one crystal structure to another.

Two allotropes of tin: gray tin ( $\alpha$ -Sn) is stable at temperatures below 13.2°C and white tin ( $\beta$ -Sn) is stable above.

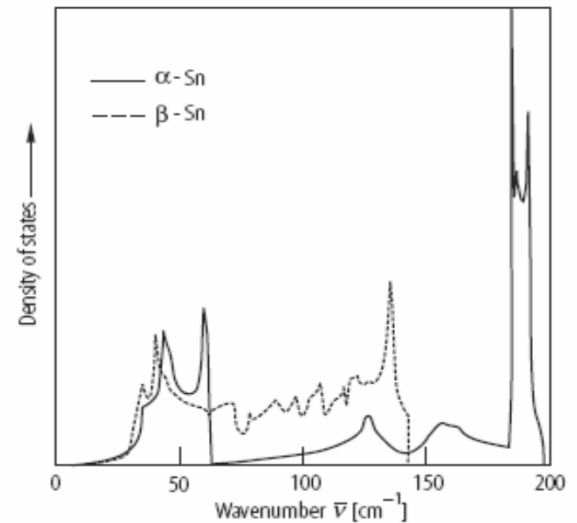
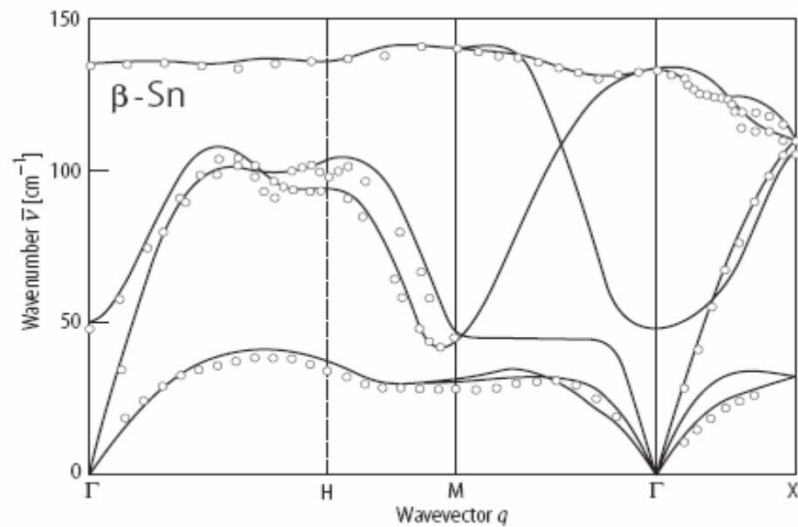
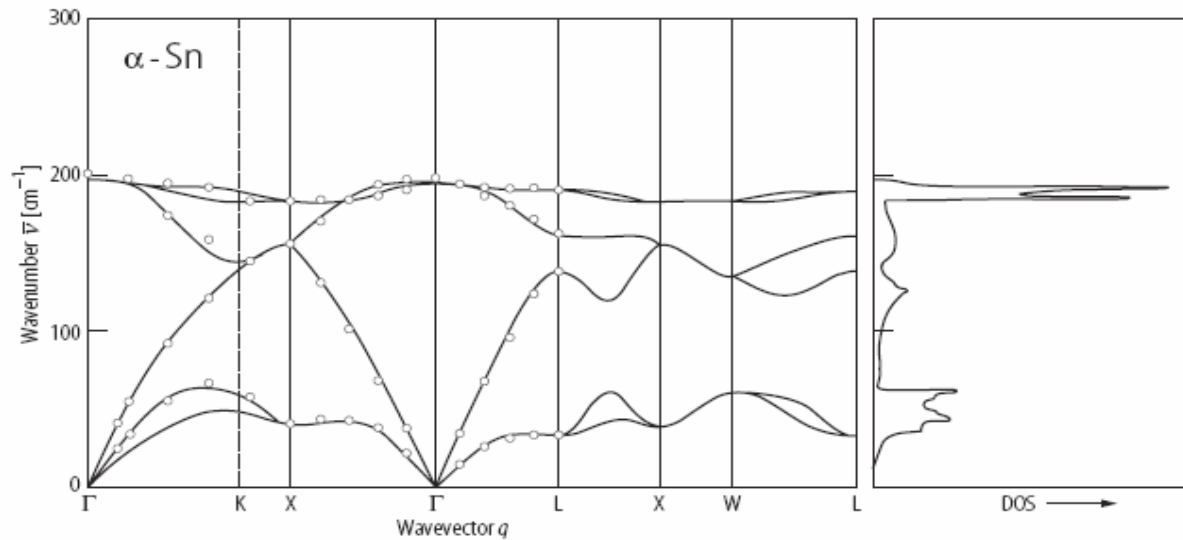
The phase with the lowest free energy prevails. (White tin can be stabilized below 13.2 C by adding impurities.)

$$F = U - TS$$

# Structural phase transition in Sn

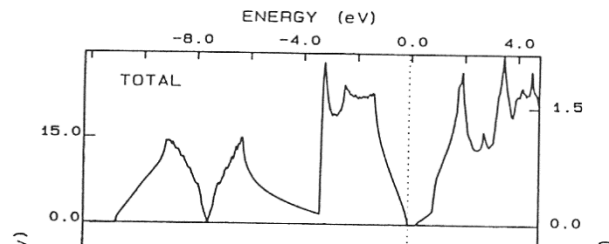
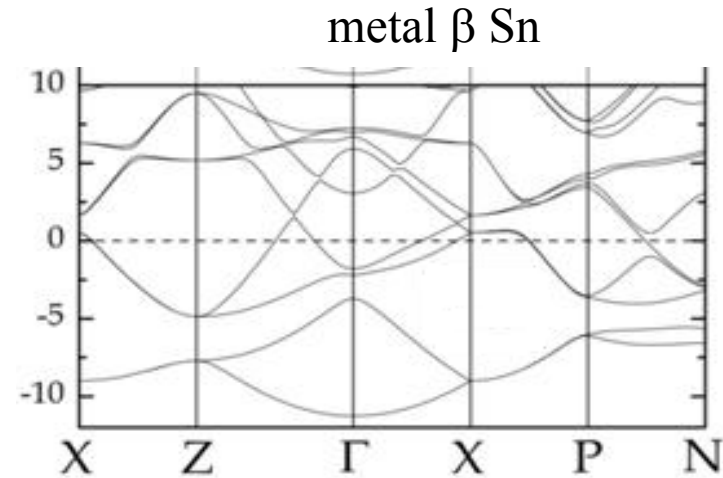
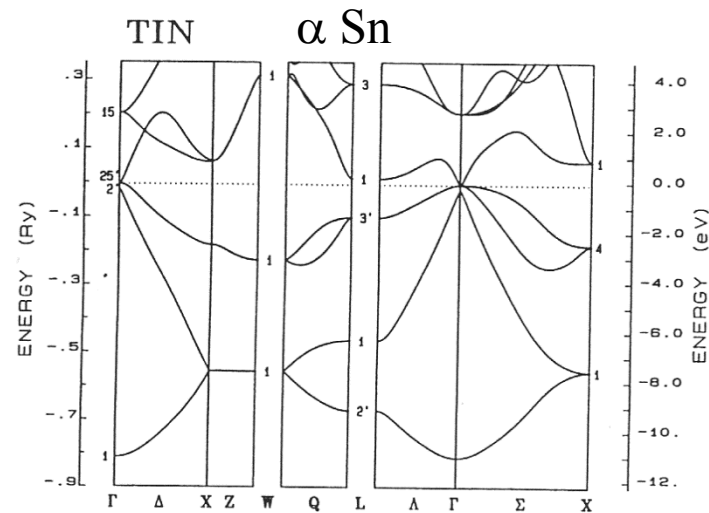
semiconductor  
diamond crystal  
structure

metal  
tetragonal  
crystal structure





# Structural phase transition in Sn



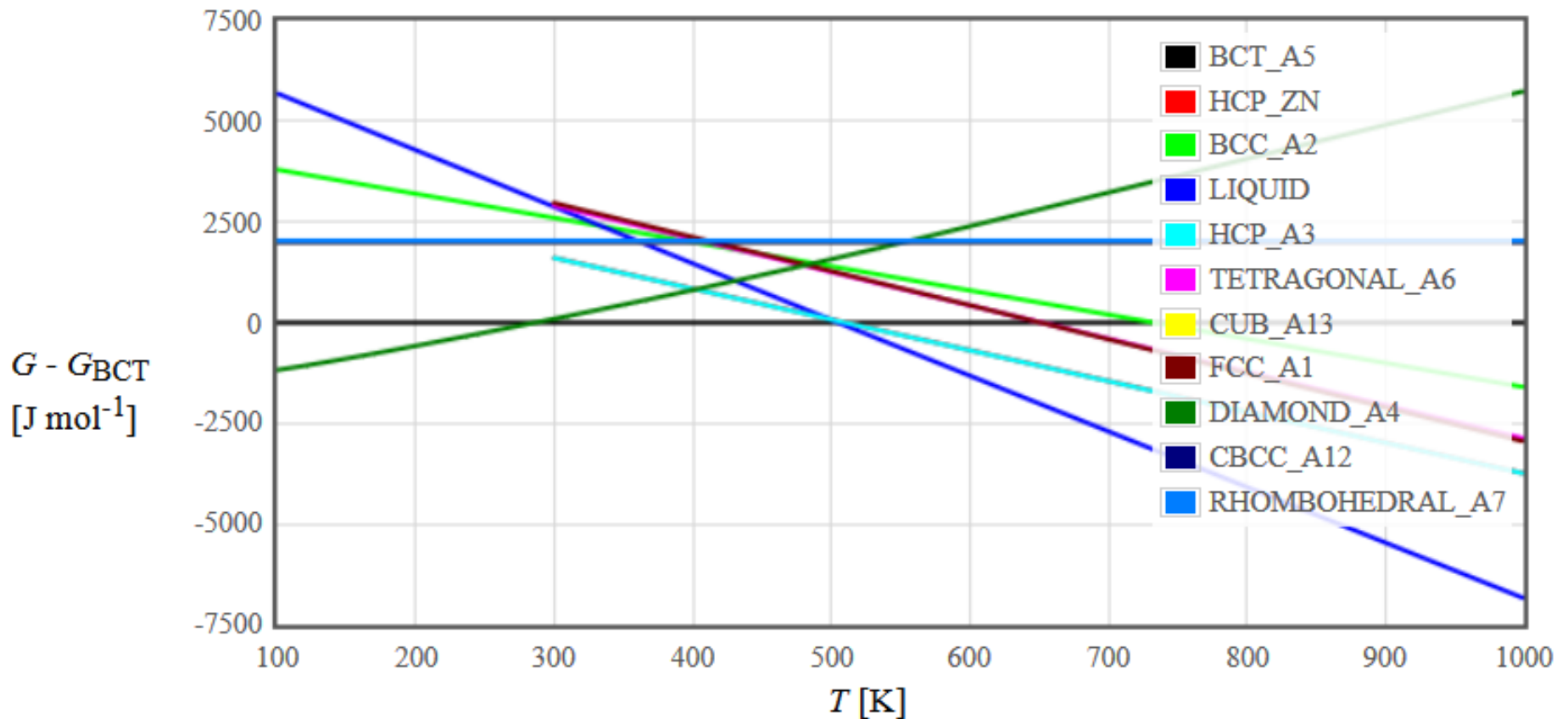
semiconductor: electrons make a negligible contribution to the entropy

$$s = \frac{\sqrt{2\pi}}{2\pi^2 \hbar^3} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right) (k_B T)^{3/2} \left(5k_B + \frac{E_g}{T}\right),$$

$$s \approx \frac{\pi^2 D(E_F)}{3} k_B^2 T$$

# Structural phase transition in Sn

metal  $\beta$  Sn = A5



<http://lampx.tugraz.at/~hadley/ss1/materials/sgte/SGTE.html>