

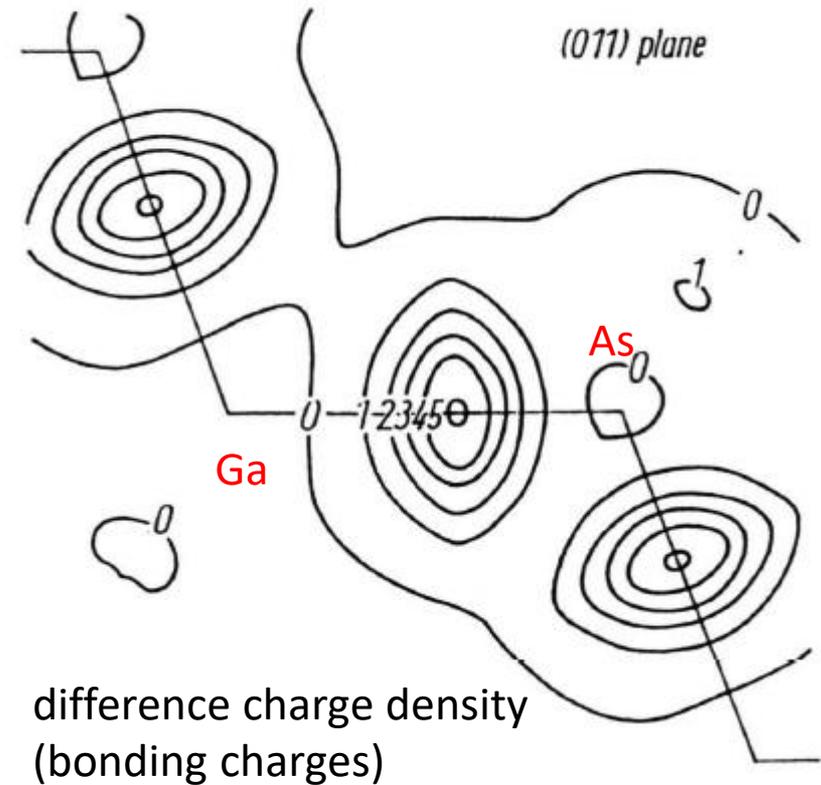
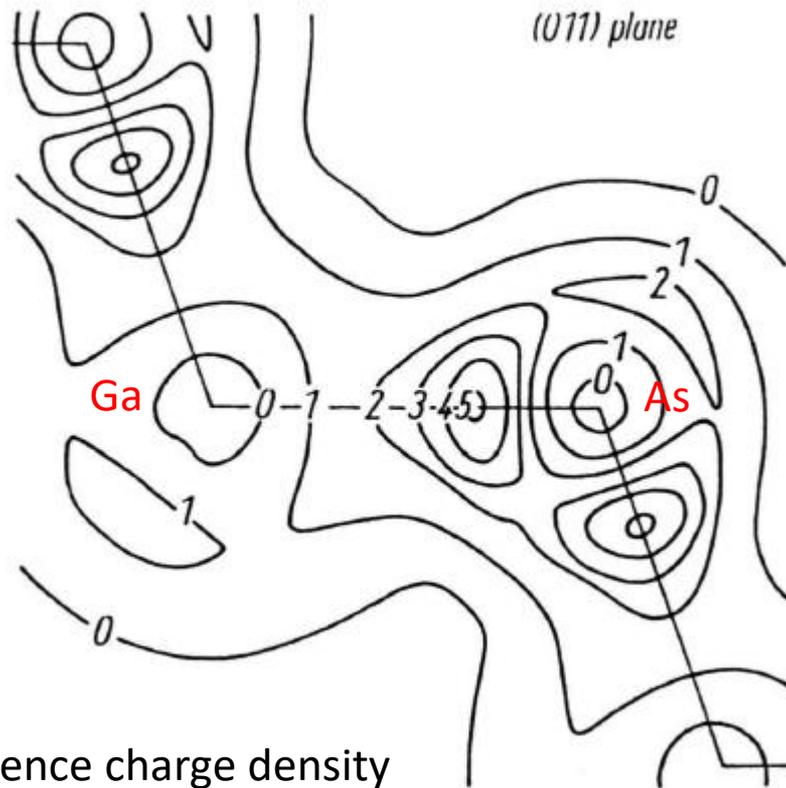
Solid state physics for Nano



Lecture 3: elasticity and elastic waves

Prof. Dr. U. Pietsch

Electron density determines elastic properties



Charge density determines the type of bond

Elasticity : general

Stress – strain relation

Linear expansion Δl under impact of external force F ,
resp, stress :

$$\sigma = F/A$$

Relative expansion, strain is $\epsilon = \Delta L/L$:

$$\sigma = E\epsilon \quad \text{Hook's law}$$

E - Young modulus

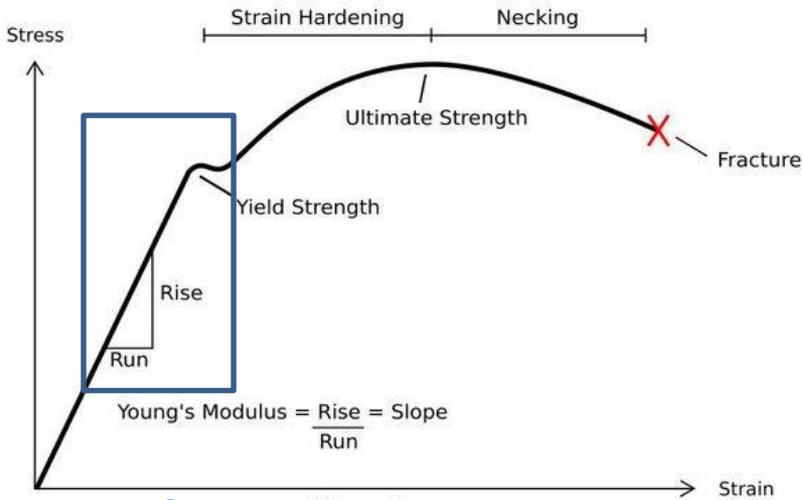
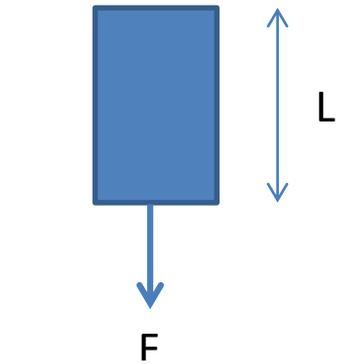
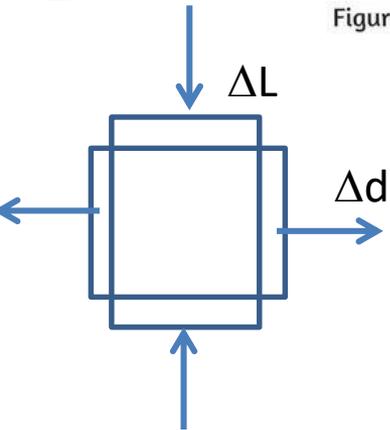


Figure 1

Transversal deformation

$$\nu = \frac{\Delta d / d}{\Delta L / L}$$

Poisson number



Elasticity : general

Change of volume

For small deformation

$$V = d^2L$$

$$\frac{\Delta V}{V} = \frac{\Delta L}{L} - 2\frac{\Delta d}{d} = \frac{\Delta L}{L}(1 - 2\nu) = \varepsilon(1 - 2\nu)$$

$$\frac{\Delta V}{V} = \frac{\sigma}{E}(1 - 2\nu)$$

Hydrostatic pressure

$$\frac{\Delta V}{V} = 3\frac{\Delta L}{L} = -\frac{3}{E}(1 - 2\nu)\Delta p$$

$$\frac{\Delta V}{V} = -\chi\Delta p$$

Compression modul K

$\chi=1/K$ - compressibility

shear stress

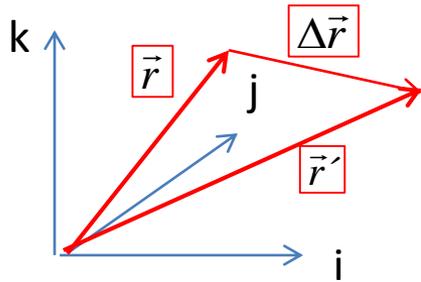
$$\sigma = \mu\theta$$

σ - shear modul

It holds the relation:

$$\frac{E}{2\mu} = 1 + \nu$$

Crystals strain



$$\vec{r} = \vec{r}' + \Delta\vec{r}$$

$$\Delta\vec{r} = u_x \vec{i} + u_y \vec{j} + u_z \vec{k}$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix}$$

Elasticity tensor
2nd rank tensor

$$\varepsilon_{11} = \frac{\partial u_x}{\partial x} \quad \varepsilon_{22} = \frac{\partial u_y}{\partial y}$$

diagonal elements

$$\varepsilon_{12} = \frac{\partial u_x}{\partial y} \quad \varepsilon_{13} = \frac{\partial u_x}{\partial z}$$

Non diagonal elements

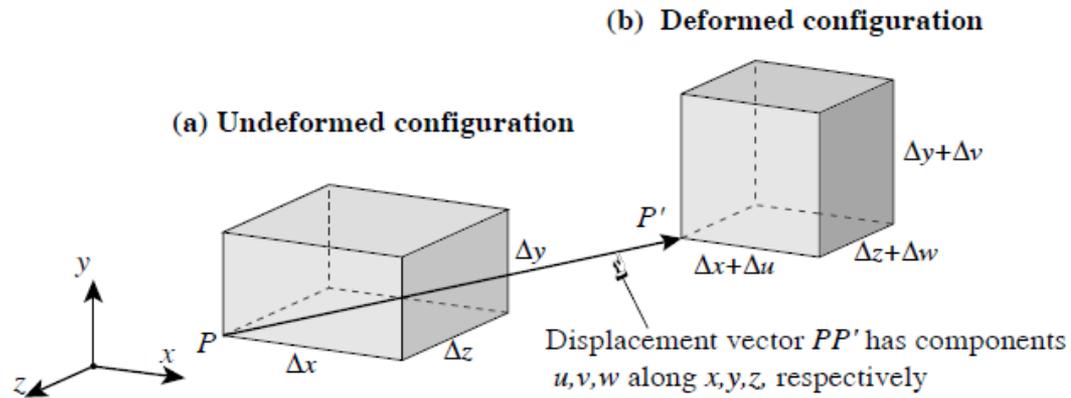
$$\varepsilon_{12} = -\varepsilon_{21} \quad \varepsilon_{23} = -\varepsilon_{32}$$

After symmetrization

$$\boldsymbol{\varepsilon}_{cub} = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{11} \end{pmatrix}$$

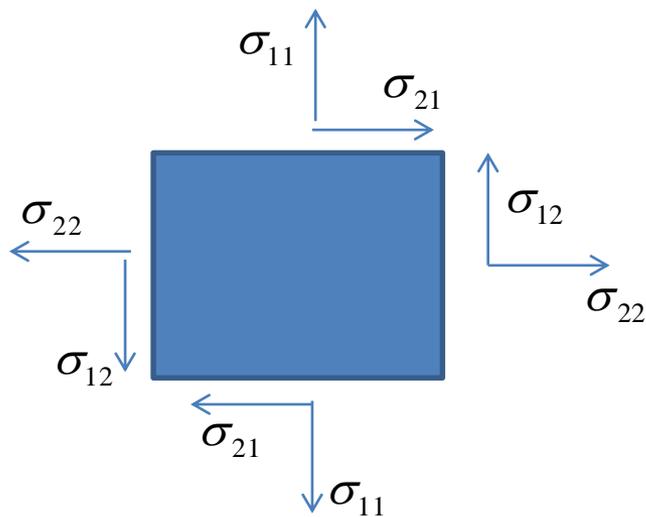
$$\boldsymbol{\varepsilon}_{tetra} = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}$$

$$\boldsymbol{\varepsilon}_{hexa} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ -\varepsilon_{21} & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}$$



$$\frac{\Delta V}{V} = \frac{V}{V_0} - 1 = (1 + \epsilon_{11})(1 + \epsilon_{22})(1 + \epsilon_{33}) - 1 \approx \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$$

stress



$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ & \sigma_{22} & \sigma_{23} \\ & & \sigma_{33} \end{pmatrix}$$

Stress tensor
2nd rank

$$\sigma_{11} \quad \sigma_{22} \quad \sigma_{33}$$

Normal stress

$$\sigma_{12} \quad \sigma_{13} \quad \sigma_{23}$$

shear stress

Hook'law for Crystals

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$$

C_{ijkl} – elastic moduli
tensor of 4th rank

$$\varepsilon_{ij} = S_{ijkl} \sigma_{kl}$$

S_{ijkl} – elastic constants
tensor of 4th rank

Number of C_{ijkl} is maximum 21, number is reducing due to symmetry

Cubic system C_{1111} C_{1122} C_{1212}

3 independent moduli

Tetragonal system

6 independent moduli

Hexagonal system

5 independent moduli

Voigt's notation

$$\begin{pmatrix} e_{11} & e_{12} & e_{13} \\ & e_{22} & e_{23} \\ & & e_{33} \end{pmatrix} \rightarrow \begin{pmatrix} e_1 & e_6 & e_5 \\ & e_2 & e_4 \\ & & e_3 \end{pmatrix} \quad \begin{array}{l} C_{1111} \rightarrow C_{11} \\ C_{1122} \rightarrow C_{12} \\ C_{1212} \rightarrow C_{44} \end{array}$$

$$\sigma_i = C_{ij} \varepsilon_j$$

Hook'law for cubic crystals

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \quad \boxed{\sigma_i = C_{ij} \varepsilon_j}$$

$$\sigma_1 = C_{11} \varepsilon_1 + C_{12} \varepsilon_2 + C_{12} \varepsilon_3$$

$$\sigma_2 = C_{12} \varepsilon_1 + C_{11} \varepsilon_2 + C_{12} \varepsilon_3$$

$$\sigma_3 = C_{12} \varepsilon_1 + C_{12} \varepsilon_2 + C_{11} \varepsilon_3$$

$$\sigma_4 = C_{44} \varepsilon_4$$

$$\sigma_5 = C_{44} \varepsilon_5$$

$$\sigma_6 = C_{44} \varepsilon_6$$

Example: hydrostatic pressure

$$\sigma = \begin{pmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{pmatrix}$$

$$\sigma_1 = c_{11}\varepsilon_1 + c_{12}\varepsilon_2 + c_{12}\varepsilon_3 = -p$$

$$\sigma_2 = c_{12}\varepsilon_1 + c_{11}\varepsilon_2 + c_{12}\varepsilon_3 = -p$$

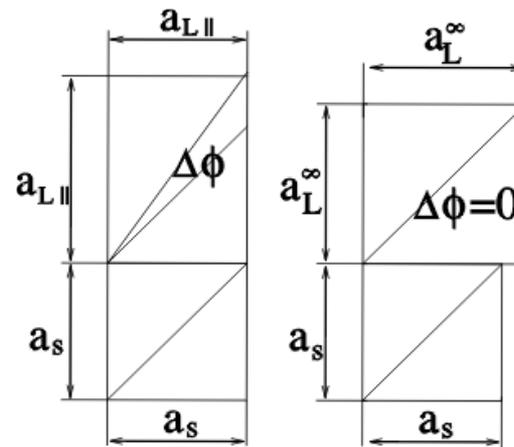
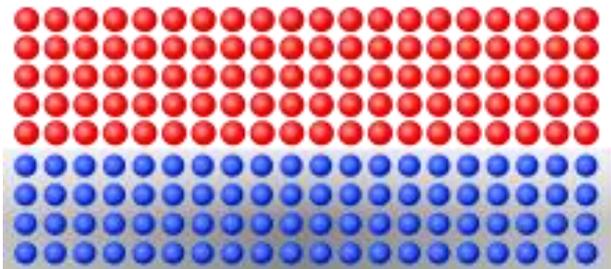
$$\sigma_3 = c_{12}\varepsilon_1 + c_{12}\varepsilon_2 + c_{11}\varepsilon_3 = -p$$

$$(c_{11} + 2c_{12})(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) = -3p$$

$$\frac{\Delta V}{V} = -\chi p$$

$$\chi = \frac{3}{c_{11} + 2c_{12}}$$

Example: Epitaxial strain



$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{||} = \frac{a_{L||} - a_{L\infty}}{a_{L\infty}} \quad \varepsilon_{\perp} = \varepsilon_{zz} = -2 \frac{c_{12}}{c_{11}} \varepsilon_{||}$$

Kubisch (2/m 3, /m 3)

e_1	e_1	$C_{11} = C_{22} = C_{33}$
e_1	$\xi \cdot e_1 = 0$	$C_{44} = C_{55} = C_{66}$
$\sqrt{2}/2 (e_1 \pm e_2)$	e_3	C_{44}
$\sqrt{2}/2 (e_1 \pm e_2)$	$(e_1 - e_2)$	$(C_{11} - C_{12})/2$
$\sqrt{2}/2 (e_1 \pm e_2)$	$(e_1 \pm e_2)$	$(C_{11} + C_{12} + 2C_{44})/2$
$\sqrt{3}/3 (e_1 + e_2 + e_3)$	$(e_1 + e_2 + e_3)$	$(C_{11} + 2C_{12} + 4C_{44})/3$
$\sqrt{3}/3 (e_1 + e_2 + e_3)$	$\xi \cdot (e_1 + e_2 + e_3) = 0$	$(C_{11} - C_{12} + C_{44})/3$

3 independent moduli

Tetragonal (4/m)

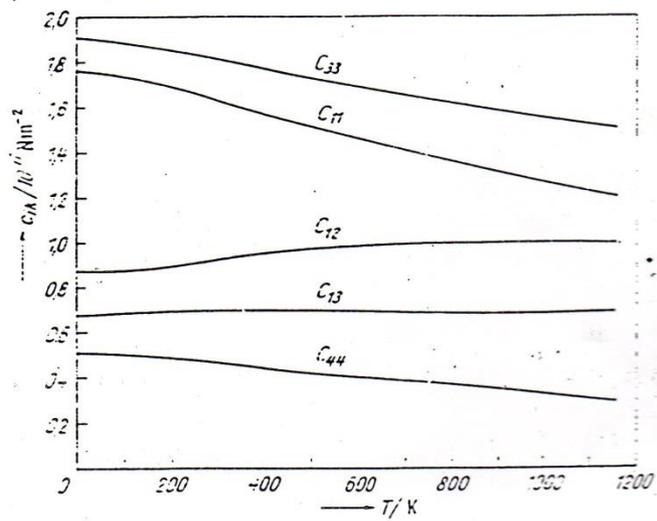
e_1	e_3	$C_{44} = C_{55}$
e_1	$\xi \cdot e_3 = 0$	$(C_{11} + C_{66})/2 \pm (1/2) \sqrt{(C_{11} - C_{66})^2 + 4C_{16}^2}$
e_3	e_3	C_{33}
e_3	$\xi \cdot e_3 = 0$	C_{44}
$\sqrt{2}/2 (e_1 \pm e_2)$	e_3	C_{44}
$\sqrt{2}/2 (e_1 \pm e_2)$	$\xi \cdot e_3 = 0$	$(C_{11} + C_{66})/2 \pm (1/2) \sqrt{(C_{12} + C_{66})^2 + 4C_{16}^2}$

6 independent moduli

Hexagonal (6/m und 6/m m) sowie ∞/m und $\infty/m m$

e_1	e_1	C_{11}
e_1	e_2	$C_{66} = (C_{11} - C_{12})/2$
e_1	e_3	$C_{44} = C_{55}$
e_3	e_3	C_{33}
e_3	$\xi \cdot e_3 = 0$	$C_{44} = C_{55}$
$\sqrt{2}/2 (e_1 \pm e_3)$	e_2	$(C_{44} + C_{66})/2$
$\sqrt{2}/2 (e_1 \pm e_3)$	$\xi \cdot e_2 = 0$	$(C_{11} + C_{33} + 2C_{44})/4$
		$\pm (1/2) \sqrt{(C_{11} - C_{33})^2/4 + (C_{13} + C_{44})^2}$

5 independent moduli



Elastic moduli depends on pressure and temperature

Comparison between isotropic and tensor components

$$\mu = c_{44} = \frac{1}{2}(c_{11} - c_{12})$$

$$c_{44} = \frac{1}{2}(c_{11} - c_{12})$$

$$E = 2 \frac{(c_{11} + 2c_{12})}{(c_{11} + c_{12})}$$

$$A = \frac{2c_{44}}{c_{11} - c_{12}} \quad \text{Cauchy relation}$$

Anisotropy ratio

Substanz	c_{11}	c_{12}	c_{44}	A
Al	1,068	0,607	0,282	1.2
C (Dia)	10,76	1,25	5,76	0.6
Cu	1,68	1,21	0,754	3.2
Ge	1,284	0,482	0,666	1.6
K	0,037	0,0314	0,0188	6.7
Si	1,657	0,639	0,796	1.6
W	5,23	2,05	1,61	1.0
InSb	0,670	0,365	0,302	2.0
GaAs	1,188	0,538	0,594	1.82
MgO	2,971	0,954	1,561	1.9
NaCl	0,494	0,127	0,128	0.7
CaF ₂	1,64	0,440	0,337	0.6

Table 11 Adiabatic elastic stiffness constants of cubic crystals at low temperature and at room temperature

C. Kittel

The values given at 0 K were obtained by extrapolation of measurements carried out down to 4 K. The table was compiled with the assistance of Professor Charles S. Smith.

Crystal	Stiffness constants, in 10^{12} dyne/cm ² (10^{11} N/m ²)			Temperature, K	Density, g/cm ³	A
	C_{11}	C_{12}	C_{44}			
W	5.326	2.049	1.631	0	19.317	1.00
	5.233	2.045	1.607	300	—	
Ta	2.663	1.582	0.874	0	16.696	1.61
	2.609	1.574	0.818	300	—	
Cu	1.762	1.249	0.818	0	9.018	3.18
	1.684	1.214	0.754	300	—	
Ag	1.315	0.973	0.511	0	10.635	2.99
	1.240	0.937	0.461	300	—	
Au	2.016	1.697	0.454	0	19.488	2.84
	1.923	1.631	0.420	300	—	
Al	1.143	0.619	0.316	0	2.733	1.21
	1.068	0.607	0.282	300	—	
K	0.0416	0.0341	0.0286	4		8.17
	0.0370	0.0314	0.0188	295		
Pb	0.555	0.454	0.194	0	11.599	3.73
	0.495	0.423	0.149	300	—	
Ni	2.612	1.508	1.317	0	8.968	2.38
	2.508	1.500	1.235	300	—	
Pd	2.341	1.761	0.712	0	12.132	2.45
	2.271	1.761	0.717	300	—	

Elastic energy

$$E = \frac{1}{2} \sum c_{ij} \varepsilon_i \varepsilon_j$$

For cubic system

$$E = \frac{c_{11}}{2} (\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) + c_{12} (\varepsilon_1 \varepsilon_2 + \varepsilon_2 \varepsilon_3 + \varepsilon_3 \varepsilon_1) + \frac{c_{44}}{2} (\varepsilon_4^2 + \varepsilon_5^2 + \varepsilon_6^2)$$

Bulk modulus
$$K = -V \left. \frac{\partial P}{\partial V} \right|_T$$

assumption
$$K = K_0 + PK_0'$$

$$V(P) = V_0 \left[1 + P \frac{K_0'}{K_0} \right]^{-1/K_0'}$$

Murnaghan equation to fit E(V) from ab-initio calculations

$$E(V) = E_0 + K_0 V_0 \left[\frac{1}{K_0' (K_0' + 1)} \left(\frac{V}{V_0} \right)^{1-K_0'} + \frac{V}{K_0' V_0} - \frac{1}{K_0' - 1} \right]$$

Ab initio calculations of electronic structure and elastic constants in AIP

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Abstract. We present an *ab initio* pseudopotential calculation within the local density approximation to determine the electronic structure and the full set of elastic constants of AIP, which have not yet been directly established experimentally. We find $C_{11} = 1.34$, $C_{12} = 0.68$ and $C_{44} = 0.70$ Mbar. We also present a study of the electronic band structure of AIP.

Ab initio calculations of the cohesive energy and the bulk modulus of Aluminium

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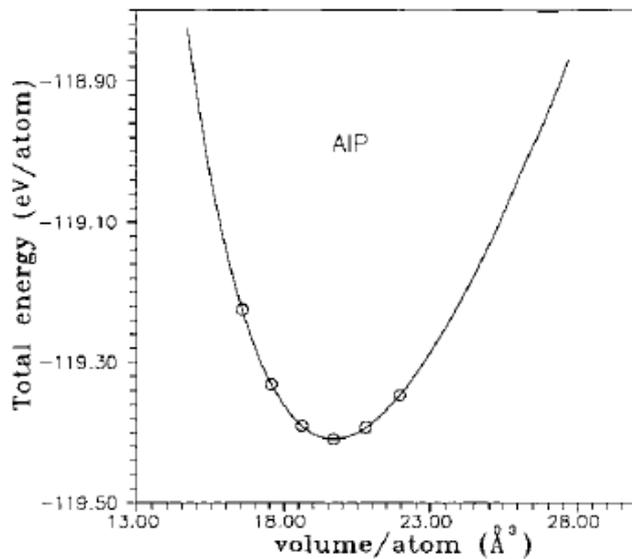
G. Rajagopal
 TCM Group, Cavendish Laboratory, Cambridge University, Madingley Road, Cambridge CB3 0HE
 (Dated: April 18, 2008)

$$B = \left(V \frac{\partial^2 E}{\partial V^2} \right) = \frac{4}{9a} \frac{\partial^2 E}{\partial a^2}$$

Table 1. Lattice constant a_0 , the elastic constants C_{ij} of AIP, the elastic constant C_{44}^0 , the optical Γ -phonon frequency ω_{Γ} , the bulk modulus B , the shear modulus C_s and the internal strain parameter ζ .

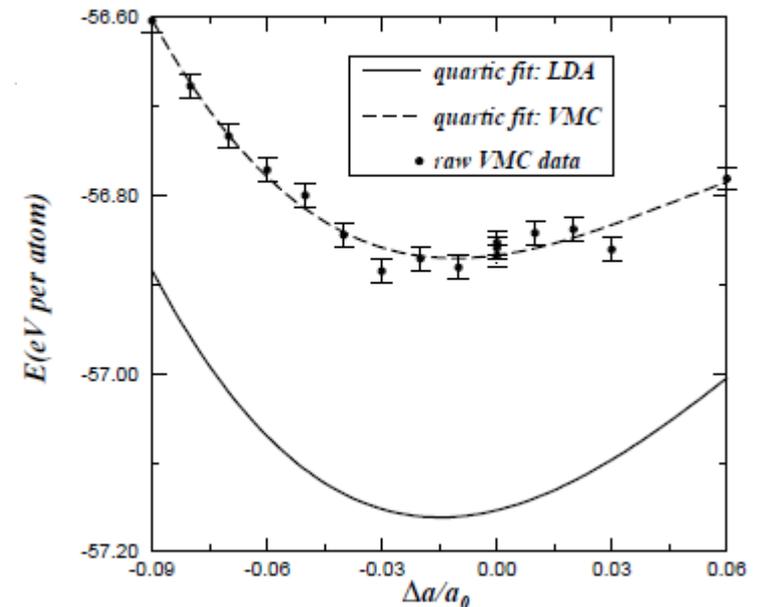
	a_0 (Å)	C_{11} (Mbar)	C_{12} (Mbar)	C_{44} (Mbar)	C_{44}^0 (Mbar)	ω_{Γ} (THz)	B (Mbar)	C_s (Mbar)	ζ
Calculation	5.40 ± 0.01	1.34 ± 0.01	0.68 ± 0.01	0.70 ± 0.02	0.919 ± 0.008	13.2 ± 0.4	0.90 ± 0.01	0.32 ± 0.01	0.53 ± 0.05
Reference [3]		1.32	0.63	0.615					
Reference [22]	5.48					13.29	0.88		
Reference [21]	5.46					13.17			

	E^c	B	B'	a	E_0^c	B_0	a_0
EXP	3.39	0.759	4.267	4.05	3.43	0.813	4.022
LDA	-	-	4.83	-	4.21	0.802	3.960
VMC	-	-	6.9(1.1)	-	3.23(8)	0.65(17)	3.970(14)

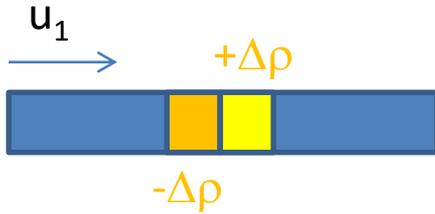


$$B = (C_{11} + 2C_{12})/3$$

$$C_s = (C_{11} - C_{12})/2$$



Elastic waves



$$\rho \frac{\partial^2 u}{\partial t^2} = \text{div } \sigma$$

$$\rho \frac{\partial^2 u_{11}}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3} = \frac{\partial \sigma_1}{\partial x_1} + \frac{\partial \sigma_6}{\partial x_2} + \frac{\partial \sigma_5}{\partial x_3}$$

$$\rho \frac{\partial^2 u_1}{\partial t^2} = c_{11} \frac{\partial \varepsilon_1}{\partial x_1} + c_{12} \left(\frac{\partial \varepsilon_2}{\partial x_1} + \frac{\partial \varepsilon_3}{\partial x_1} \right) + c_{44} \left(\frac{\partial \varepsilon_6}{\partial x_2} + \frac{\partial \varepsilon_5}{\partial x_3} \right)$$

$$\rho \frac{\partial^2 u_1}{\partial t^2} = c_{11} \frac{\partial^2 u_1}{\partial x_1^2} + c_{44} \left(\frac{\partial^2 u_1}{\partial x_2^2} + \frac{\partial^2 u_1}{\partial x_3^2} \right) + (c_{12} + c_{44}) \left(\frac{\partial^2 u_2}{\partial x_1 \partial x_2} + \frac{\partial^2 u_3}{\partial x_1 \partial x_3} \right)$$

$$\rho \frac{\partial^2 u_2}{\partial t^2} = c_{11} \frac{\partial^2 u_2}{\partial x_2^2} + c_{44} \left(\frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_3^2} \right) + (c_{12} + c_{44}) \left(\frac{\partial^2 u_1}{\partial x_1 \partial x_2} + \frac{\partial^2 u_3}{\partial x_2 \partial x_3} \right)$$

$$\rho \frac{\partial^2 u_3}{\partial t^2} = c_{11} \frac{\partial^2 u_3}{\partial x_3^2} + c_{44} \left(\frac{\partial^2 u_3}{\partial x_1^2} + \frac{\partial^2 u_3}{\partial x_2^2} \right) + (c_{12} + c_{44}) \left(\frac{\partial^2 u_1}{\partial x_1 \partial x_3} + \frac{\partial^2 u_2}{\partial x_2 \partial x_3} \right)$$

For [100]

$$u_1 = u_0 e^{i(\omega t - k_1 x_1)} \quad \frac{\partial^2 u_1}{\partial x_1^2} = -k_1^2 u_1 \quad -\sigma \omega^2 = -c_{11} k_1^2 \Rightarrow \text{--- } v_l^{[100]} = \frac{\omega_l}{k_l} = \sqrt{\frac{c_{11}}{\rho}}$$

$$\frac{\partial^2 u_1}{\partial t^2} = -\omega^2 u_1 \quad -\sigma \omega^2 = -c_{44} k_t^2 \Rightarrow \text{--- } v_t^{[100]} = \frac{\omega_t}{k_t} = \sqrt{\frac{c_{44}}{\rho}} = \sqrt{\frac{c_{11} - c_{12}}{\rho}}$$

For [110]

$$v_l^{[110]} = \frac{\omega_l}{k_l} = \sqrt{\frac{c_{11} + c_{12} + 2c_{44}}{2\rho}}$$

$$v_t^{[110]} = \frac{\omega_t}{k_t} = \sqrt{\frac{c_{44}}{\rho}} \neq \sqrt{\frac{c_{11} - c_{12}}{\rho}}$$

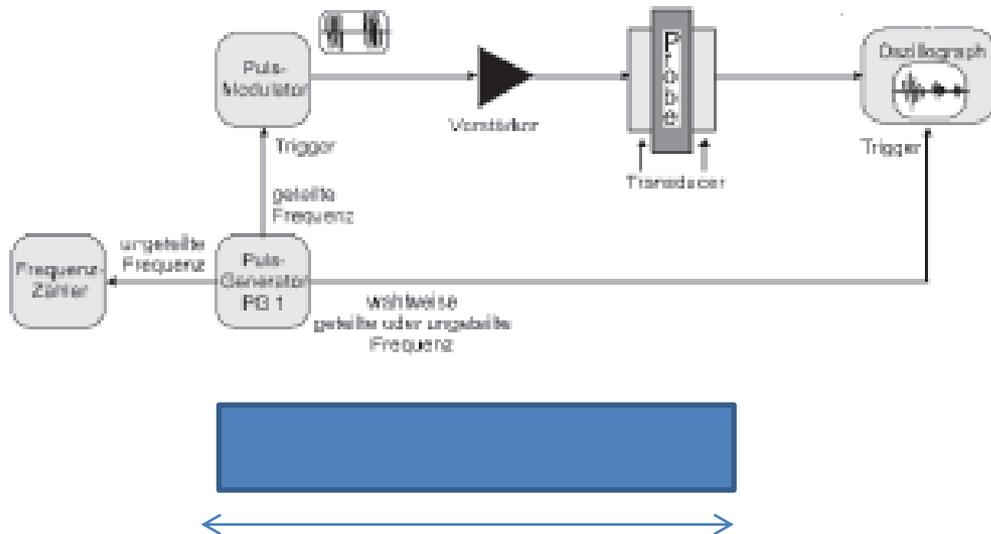
For [111]

$$v_l^{[111]} = \frac{\omega_l}{k_l} = \sqrt{\frac{c_{11} + 2c_{12} + 4c_{44}}{3\rho}}$$

$$v_t^{[110]} = \frac{\omega_t}{k_t} = \sqrt{\frac{c_{11} - c_{12} + c_{44}}{3\rho}}$$

Measure elastic constants from sound velocity

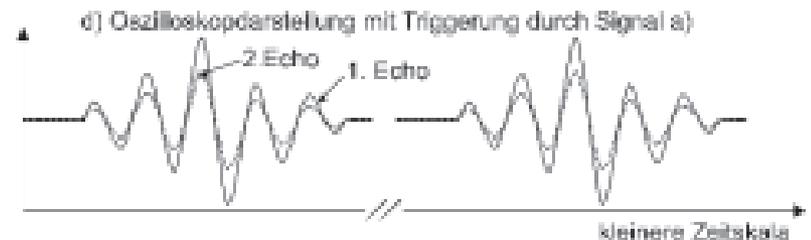
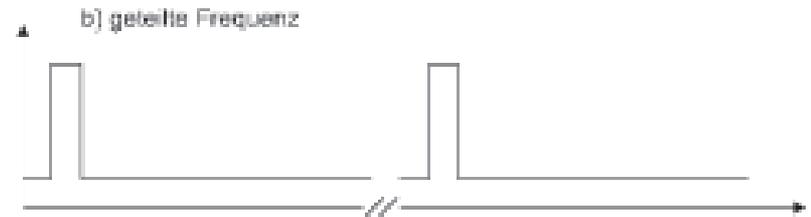
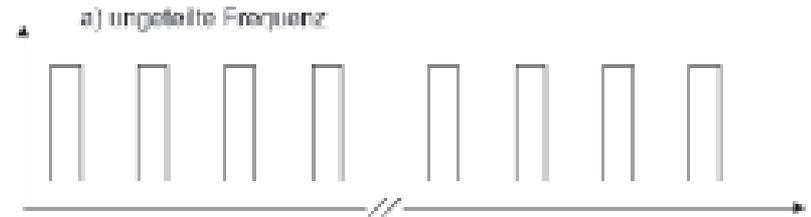
Measurement of elastic moduli by Impuls-echo-overlap method



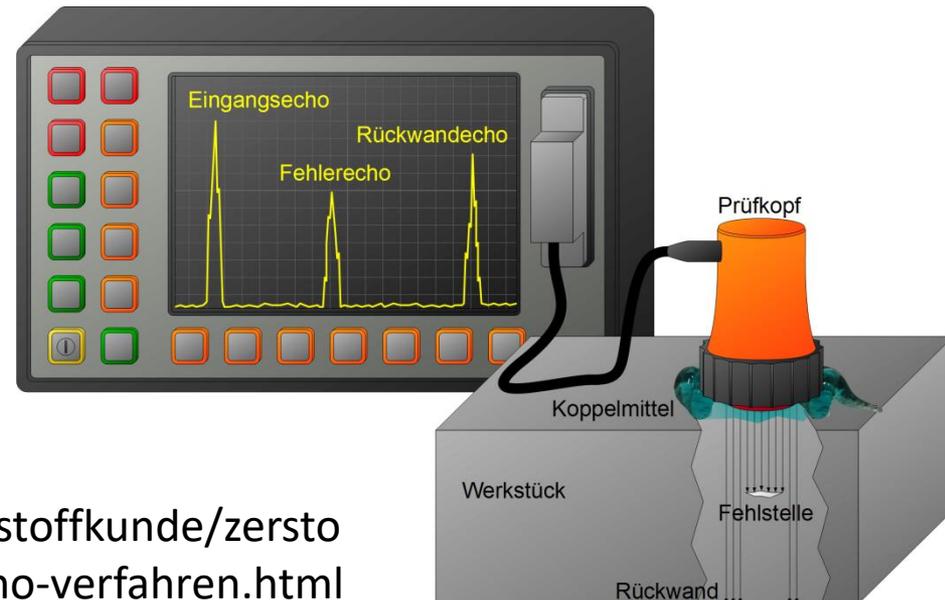
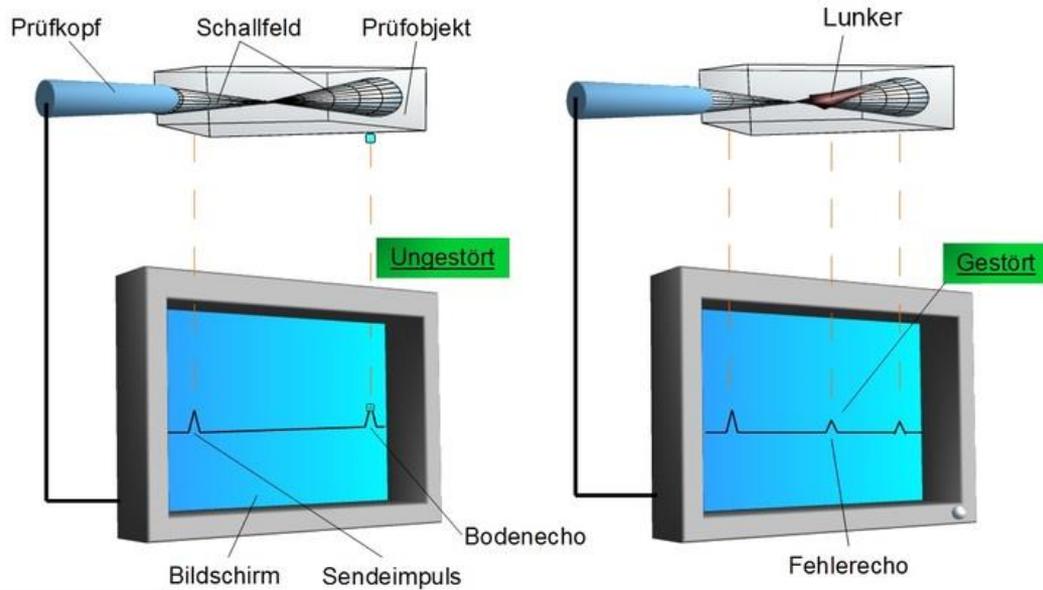
L

$$v = \frac{2L}{t}$$

$$\Delta v = \sqrt{\frac{2(\Delta L)^2}{t} + \frac{2L(\Delta t^2)}{t^2}}$$



Impuls-Echo Verfahren zur Defektanalyse



<http://www.ahoefer.de/maschinenbau/werkstoffkunde/zerstoerungsfreie-werkstoffpruefung/30-impuls-echo-verfahren.html>

Impuls-Echo Verfahren zur Defektanalyse

Substanz	c [m/s]	Dämpfung dB / cm
Glas	5900	
Eisen (Stahl)	5200	
PVC	2010	
Fett	1470	0,5
Muskel	1568	2
Knochen (kompakt)	3600	4 - 10
Wasser (20 C)	1492	0,002
Luft (NN)	331	

Typical values of sound velocity and damping of ultrasound (f= 1 MHz) for different materials

In case diameter is large compared to wave length of ultrasound:

n

$$c_{\text{Festkörper, longitudinal}} = \sqrt{\frac{E(1-\mu)}{\rho(1-\mu-2\mu^2)}}$$

Sound velocity in a thin long strick

$$c_{\text{longitudinal}} = \sqrt{\frac{E}{\rho}}$$

Sonographie – Ultraschallverfahren in der Medizin

Aus der Differenz der gesendeten und empfangenen Ultraschallwellen erstellt der Computer ein Bild. Je besser Gewebe reflektiert, umso heller wird es abgebildet. Die Reflektionsstärke ist abhängig von der Dichte des untersuchten Gewebes. Besonders gut sichtbar sind Knochen. Diese reflektieren den Schall am besten. Im Bild wird Knochenmaterial genau wie auf einem Röntgenbild weiß dargestellt. Wasser- und blutreiche Gewebe haben unterschiedliche Schall- dichten und werden deswegen in verschiedenen Graustufen ausgewertet.



Ultraschallaufnahme eines Fötus in der Gebärmutter.

B-Bild-Sonographie (B-Mode): Die gewonnenen Echo-Signale werden als zweidimensionale Schnittbilder in Graustufen sichtbar gemacht. Der B-Mode ist momentan die am weitesten verbreitete Variante der Ultraschalluntersuchung in der Medizin.

M-Mode: Damit lassen sich Bewegungsabläufe (beispielsweise der Herzklappenrhythmus) von sich bewegenden Organen abbilden. Diese Bewegungen werden eindimensional in Diagrammen wiedergegeben.

Echokardiographie: Dieses Verfahren wird für Strömungsmessungen im Herzen und in Gefäßen verwendet. Das reflektierte Echo der sich bewegenden roten Blutkörperchen wird elektronisch hörbar gemacht und als Kurve aufgezeichnet.

Dopplersonographie oder Duplex-Sonographie: Bei dieser Untersuchung wird der Blutstrom akustisch und bildlich dargestellt. Unterstützt wird dieses Verfahren mit einer Farbkodierung. Der Blutfluss zum Schallkopf hin und von ihm weg wird in verschiedenen Farben markiert. Veränderungen der Flussgeschwindigkeiten können mit diesem Verfahren diagnostiziert werden.

3D-Ultraschall: Dabei handelt es sich um ein Schnittbild zweidimensional aufgenommener Bildebenen. Der Rechner wertet die zweidimensionalen Bilder aus und kann so eine dritte Bildebene errechnen. Bei diesen Verfahren

Kontrastmittel-Ultraschall: Diese noch recht neue Methode macht die Durchblutung von Gefäßen und Organen und die Versorgung von Tumoren sichtbar. Die eingesetzten Kontrastmittel sind besser verträglich als solche, die bei Röntgen-, CT- oder MRT-Untersuchungen eingesetzt werden.