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Shear modulus of cubic crystals

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Модуль сдвига кубических кристаллов

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For cubic crystals the variability of the shear modulus is analyzed. Extreme values of the shear modulus and their directions are determined. It is shown that the dimensionless shear modulus depends on the crystal orientation and a positive dimensionless elastic parameter. The value of this parameter specifies, in particular, the ratio of maximum and minimum values of the shear modulus. The lists of the extreme values of shear moduli of various cubic crystals with negative Poisson's ratio, ordered by the magnitude of the elastic parameter, are given.

Keywords: Shear modulus, cubic crystal, auxetic.

Для кубических кристаллов проанализирована изменчивость модуля сдвига. Определены экстремальные значения модуля и их направления. Показано, что безразмерный модуль сдвига зависит от ориентации кристаллов и одного положительного безразмерного упругого параметра. Величиной этого параметра определяется, в частности, отношение максимального и минимального значений модуля сдвига. При ограничении кристаллами с отрицательными коэффициентами Пуассона даны упорядоченные по величине упругого параметра списки экстремальных значений модулей сдвига различных кубических кристаллов.

Ключевые слова: модуль сдвига, кубический кристалл, ауксетик.

1. Introduction

Young's modulus, Poisson's ratio and shear modulus for isotropic materials are constant. For anisotropic materials elastic properties depend on the orientation of the test specimens.

In this paper we analyze the variability of shear modulus of cubic auxetics with the change in the orientation angles of tensile specimens. There are used experimental data for the elasticity coefficients of cubic crystals with negative Poisson's ratio (auxetics), contained in [1] and in [2,3].

In the linear elasticity the shear modulus $G(\mathbf{n},\mathbf{m})$ is defined by two unit vectors $\mathbf{n}$ and $\mathbf{m}$ [4]

$$G^{-1}(\mathbf{n},\mathbf{m}) = 4s_{ijkl}n_i m_j n_k m_l\,.$$

Here, vector $\mathbf{n}$ - unit vector normal to the slip plane, and vector $\mathbf{m}$ - unit vector in the direction of slip. Below, components of the fourth-rank tensor s_{ijkl} in the crystallographic coordinate system are replaced by compliance matrix coefficients s_{mn} [5].

2. Extreme values of the shear modulus for cubic crystals

The shear modulus in the particular case of cubic crystals takes the form

$$G(\mathbf{n},\mathbf{m}) = \frac{1}{s_{44} + 2(s_{11} - s_{12} - 0.5s_{44})N(\mathbf{n},\mathbf{m})}\,, \qquad (1)$$

$$N(\mathbf{n},\mathbf{m}) \equiv 2\left(n_1^2 m_1^2 + n_2^2 m_2^2 + n_3^2 m_3^2\right).$$

Here $N(\mathbf{n},\mathbf{m})$ is a function only of mutually orthogonal unit vectors $\mathbf{n}$ and $\mathbf{m}$. Its form does not depend on the elastic properties of crystals.

Also we rewrite the shear modulus as a function of Euler angles. Mutually orthogonal unit vectors $\mathbf{n}$ and $\mathbf{m}$ are represented in the Euler angles φ, θ, ψ as follows

$$\mathbf{n} = \begin{pmatrix} \sin\varphi\sin\theta \\ -\cos\varphi\sin\theta \\ \cos\theta \end{pmatrix},$$

$$\mathbf{m} = \begin{pmatrix} -\sin\varphi\cos\theta\cos\psi - \cos\varphi\sin\psi \\ \cos\varphi\cos\theta\cos\psi - \sin\varphi\sin\psi \\ \sin\theta\cos\psi \end{pmatrix}.$$

Restrictions are valid for components of these vectors

$$n_1^2 + n_2^2 + n_3^2 = 1, \quad m_1^2 + m_2^2 + m_3^2 = 1,$$

$$n_1 m_1 + n_2 m_2 + n_3 m_3 = 0. \qquad (2)$$

Expression of the shear modulus for cubic crystals (1) through the Euler angles can be rewritten as

$$G(\varphi,\theta,\psi) = \frac{1}{s_{44} + 2(s_{11} - s_{12} - 0.5 s_{44}) N(\varphi,\theta,\psi)},$$

$$N(\varphi,\theta,\psi) = \left\{3\cos^2\theta\cos^2\psi + +(\cos\theta\cos2\varphi\cos\psi - \sin2\varphi\sin\psi)^2\right\}\sin^2\theta.$$

Thus, we have two different parameterizations of the function N. Analysis of the function $N(\mathbf{n},\mathbf{m})=N(\varphi,\theta,\psi)$ shows that it is limited [6]

$$0 \le N(\mathbf{n},\mathbf{m}) = N(\varphi,\theta,\psi) \le 1. \qquad (3)$$

The dependence of the shear modulus of the elastic coefficients and the angular variables is conveniently written in dimensionless form

$$\frac{1}{s_{44}G} = 1 + (P-1)N(\varphi,\theta,\psi),$$

$$P \equiv 2\frac{s_{11} - s_{12}}{s_{44}} = 2\frac{c_{44}}{c_{11} - c_{12}}.$$

Here, the elastic dimensionless parameter P is expressed through the compliance modules or the stiffness coefficients. Due to the thermodynamic restrictions of the compliance modules $s_{11} - s_{12} > 0$, $s_{44} > 0$ the parameter P is nonnegative. Accounting for relations (3), we find the following constraints on the dimensionless shear modulus $s_{44}G$

$$0 < P < 1: \quad 0 < P < \frac{1}{s_{44}G} < 1,$$

$$1 < P: \quad 1 < \frac{1}{s_{44}G} < P.$$

They are shown schematically in Fig. 1.

It follows that the value of a parameter P determines the relative magnitude of the maximum and minimum of the shear modulus. At $P>1$ ratio G_{max}/G_{min} is equal to P, and at $P < 1$ this ratio is equal to $1/P$. At the same time, the minimum value G_{min} is always positive. All this is reflected in Tables 1-4. Data on the elastic properties of cubic crystals in [1] are too numerous. Therefore, we are confined ourselves here only by cubic auxetics. Moreover, in Tables 3 and 4 we adopted the restriction by auxetics with large values of the elastic dimensionless parameter (at $P \ge 10$) and the relative small values of this parameter ($1<P\le2.5$). All data are arranged in accordance with the value of dimensionless parameter P, and hence the ratio G_{max}/G_{min}. Table 1 contains the results for the

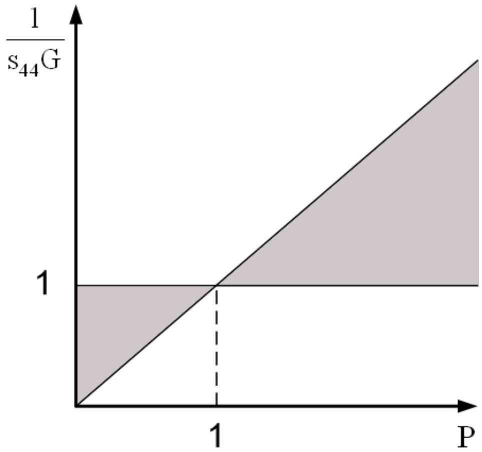

Fig. 1. Changing the range of inverse values of the dimensionless shear modulus with a change in the value of the dimensionless elastic parameter. Region of possible values $(s_{44}G)^{-1}$ is shaded.

Table 1

The values of the compliance modulus s_{44}, dimensionless parameter P and maximum and minimum values of the shear modulus of complete auxetics.

Cubic crystal	s_{44}, TPa^{-1}	P	s_{44}^{-1}, GPa	$\left(2(s_{11}-s_{12})\right)^{-1}$, GPa
Ba	98.9	2.38	10.1	4.25
	105	4.15	9.52	2.29
$Sm_{0.7}Y_{0.3}S$	33.3	0.32	30.0	92.6
	32.3	0.34	31.0	91.1
$Sm_{0.75}Y_{0.25}S$	34.5	0.38	29.0	76.9
	33.3	0.35	30.0	84.7
	33.3	0.35	30.0	84.7
$Sm_{0.75}La_{0.25}S$ [10]	35.71	0.48	28.0	58.5
$Sm_{0.65}La_{0.35}S$ [10]	27.78	0.92	36.0	39.0
$Sm_{0.75}Tm_{0.25}S$ [10]	27.03	0.61	37.0	60.5

Table 2

The values of the compliance modulus s_{44}, dimensionless parameter P and maximum and minimum values of the shear modulus of partial auxetics with $0<P<1$.

Cubic crystal	s_{44}, TPa^{-1}	P	s_{44}^{-1}, (G_{min},GPa)	$\left(2(s_{11}-s_{12})\right)^{-1}$, ($G_{max}$,GPa)
USe	67.6	0.12	14.8	128
UTe	83.3	0.16	12.0	72.8
USb	56.2	0.17	17.8	102
TmSe	38.5	0.21	26.0	125
$Tm_{0.99}Se$	37	0.23	27.0	118
SnTe	81	0.23	12.3	53.8
GeTe-SnTe	80.6	0.24	12.4	52.1
ReO_3	16.4	0.25	61.0	243
$Sm_{0.90}La_{0.10}S$ [10]	41.67	0.33	24.0	72.6
SmB_6	12.82	0.37	78.0	211
$Sm_{0.85}Tm_{0.15}S$ [10]	38.46	0.48	26.0	54.5
FeS_2	8.79	0.51	114	222

complete auxetics, which have a negative Poisson's ratio for any orientations of the crystals. In Tables 2-4 the results are presented for partial auxetics, i.e. for crystals with negative Poisson's ratio for some orientations, and positive for others. The number of partial auxetics in Tables 2-4 under constraints 0<P≤2.5, P≥10, significantly less than the total number of partial cubic auxetics (over 350 [7]). Large magnitude $G_{max}/G_{min}=P$ were in crystalline alloys InTl. For them, under certain conditions, this ratio exceeds 10^3.

3. Extreme directions for which the shear modulus is s_{44}^{-1}

The analysis will begin with three particular cases where the unit vector **n** has only one nonzero component.

1) $n_1^2=1,\ \ n_2=n_3=0$. This corresponds to φ=0= π/2 and $\mathbf{m}^T=(0,-\sin\psi,\cos\psi)$; the equality $N(\pi/2,\pi/2,\psi)=0$ is fulfilled.

Table 3

The values of the compliance modulus s_{44}, dimensionless parameter *P* and maximum and minimum values of the shear modulus of partial auxetics with 1<*P*≤2.5.

Cubic crystal	s_{44}, TPa^{-1}	*P*	s_{44}^{-1}, (G_{max}, GPa)	$(2(s_{11}-s_{12}))^{-1}$ (G_{min},GPa)
LiD	22	1.76	45.5	25.8
LiH	22	1.78	45.5	25.5
FeCoCrMo (25at%Co, 30at%Cr, 3.4at%Mo)	8.7	1.82	115	63.3
LiF	15.8	1.89	63.3	33.4
SiC	3.98	2.11	251	119
	4.29	2.20	233	106
$MgO{\cdot}3.5Al_2O_3$	6.35	2.14	157	73.4
	6.31	2.16	158	73.4
	6.36	2.18	157	72.0
FeCr (19.43at%Cr)	8.97	2.15	111	51.9
$MgO{\cdot}2.61Al_2O_3$	6.35	2.17	157	72.5
CuAu (80at%Au)	24.09	2.18	41.5	19.0
$Ge_{0.72}Si_{0.28}$	11.7	2.21	85.5	38.8
$CeSn_3$	23.2	2.23	43.1	19.3
$C_{10}H_{16}$	291	2.26	3.44	1.52
	21	3.47	47.6	13.7
	226	2.70	4.42	1.64
ZnSe	24.9	2.32	40.2	17.3
$Ag_6Sn_4P_{12}Ge_6$	18.9	2.36	52.9	22.4
$Sr(NO_3)_2$	63.1	2.38	15.8	6.65
PdRh (20at%Rh)	11.08	2.40	90.3	37.6
ZnS	22.5	2.41	44.4	18.5
$MgAl_2O_4$	6.49	2.42	154	63.7
CdTe	49.4	2.43	20.2	8.33
Fe	8.57	2.45	117	47.6
AlNi (47.5%Ni)	9.44	2.45	106	43.3
LaAg	47.8	2.45	20.9	8.55
$ZnFe_2O_4$	7.41	2.50	135	54.0

Table 4

The values of the compliance modulus s_{44}, dimensionless parameter *P* and maximum and minimum values of the shear modulus of partial auxetics with *P*≥10.

Cubic crystal	s_{44}, TPa^{-1}	*P*	s_{44}^{-1}, (G_{max}, GPa)	$(2(s_{11}-s_{12}))^{-1}$ (G_{min},GPa)
$Au_{20}Cu_{33}Zn_{47}$	16.6	10.0	60.2	6.00
CuZn (46at%Zn)	12.5	10.1	80.0	7.94
CuAlNi (Cu-14wt% Al-4.1wt%Ni)	10.4	10.2	96.2	9.40
CuZn (43at%Zn)	13	10.4	76.9	7.40
CuZn (47.8at%Zn)	12.5	10.8	80.0	7.94
$Cu_{30}Ni_{20}Zn_{50}$	11.6	10.9	86.2	7.90
β_1-AgCd (47.9at%Cd)	19.6	11.2	51.0	4.55
InTl (39.06%Tl)	115	11.5	8.70	0.76
$Cu_{66.5}Zn_{20.8}Al_{12.7}$	11.8	12.0	84.7	7.05
CuAlZn (Cu-17at%Al-14.3at%Zn)	12.07	12.0	82.9	6.89
CuAlNi (Cu-14.5wt%Al-3.15wt%Ni)	9.7	12.1	103	8.50
$Au_{23}Cu_{30}Zn_{47}$	18	12.3	55.6	4.50
$Cu_{25}Ni_{25}Zn_{50}$	11.4	12.4	87.7	7.10
$Au_{30}Cu_{23}Zn_{47}$	17.2	12.9	58.1	4.50
$Mn_{85.3}Ni_{8.8}C_{5.9}$	9.78	13.6	102	7.51
InTl (35.15at%Tl)	115	14.6	8.70	0.59
$Cu_{67.7}Zn_{19.4}Al_{12.9}$	11.6	14.8	86.2	5.81
AlNi (60%Ni)	8.31	15.0	120	8.01
$CuAuZn_2$	18.9	17.8	52.9	2.98
InTl (30.16at%Tl)	118	22.5	8.47	0.38
$NiCr_2O_4$	17.3	23.1	57.8	2.50
InTl (27at%Tl, 290 K) [11]	119	24.0	8.40	0.35
InTl (27at%Tl)	119	25.8	8.40	0.33
FePd (28at%Pd)	12.5	26.7	80.0	2.99
InTl(28.13at%Tl)	120	28.6	8.33	0.29
InTl (25at%Tl)	126	34.5	7.94	0.23
InTl (27at%Tl, 200 K) [11]	110	90.9	9.09	0.10
InTl (27at%Tl, 125 K) [11]	105	1905	9.52	0.005

2) $n_2^2=1,\ \ n_1=n_3=0$. In this case φ=0, θ=π/2 and $\mathbf{m}^T=(-\sin\psi,0,\cos\psi)$, and performed $N(0,\pi/2,\psi)=0$

3) $n_3^2=1,\ \ n_1=n_2=0$. This is attained at $\theta=0$ with no restrictions on φ. Then the cross-vector has the form $\mathbf{m}^T=(-\sin(\varphi+\psi),\cos(\varphi+\psi),0)$ and performed $N(\varphi,0,\psi)=0$.

In three other special cases only one component of the unit vector **n** is zero.

4) n_1=0 , n_2≠0, n_3≠0. This corresponds to φ=0. Conditions **n·m**=0, N(**n**,**m**)=0 take the form of the system of equations $-m_2\sin\theta + m_3\cos\theta = 0$, $m_2^2\sin^2\theta + m_3^2\cos^2\theta = 0$, which has only the trivial solution m_2=m_3=0, and ψ=π/2 и m_1=-1. The condition $N(0,\theta,\pi/2)$=0 is satisfied.

5) n_2=0, n_1≠0, n_3≠ 0. This is true at φ=π/2. Similarly to the previous case the two components m_1, m_3 of the vector **m** are zero, so that ψ=π/2 and m_2=-1. The condition $N(\pi/2,\theta,\pi/2)$=0 is satisfied.

6) n_3=0, n_1≠0, n_2≠ 0 is possible at θ=π/2. Similarly to the previous case m_1=m_2=0, ψ=0 and m_3=1. The condition $N(\varphi,\pi/2,0)$=0 is satisfied.

Finally, in the case

7) n_1≠0, n_2≠0, n_3≠0 the absence of nontrivial result for vector m follows from the condition N(**n**,**m**)=0. Thus at this most general orientation n the extreme s_{44}^{-1} of the shear modulus is not achieved.

4. Extreme directions for which the shear modulus is $\left(2s_{11}-2s_{12}\right)^{-1}$

This value of the shear modulus is achieved under the condition N(**n**,**m**)=1. We turn again to discuss the sequence of individual cases, as in the previous section.

In three cases, with one nonzero component of the vector **n**

1) $n_1^2 = 1,\ \ n_2 = n_3 = 0$ corresponds to φ=θ=π/2. At the same time $N(\pi/2,\pi/2,\psi)$ becomes zero and thus extreme $\left(2s_{11}-2s_{12}\right)^{-1}$ is impossible.

2) $n_2^2 = 1,\ \ n_1 = n_3 = 0$ corresponds to φ=0, θ=π/2, that also leads to the vanishing of the function $N(0,\pi/2,\psi)$ and extreme $\left(2s_{11}-2s_{12}\right)^{-1}$ is impossible.

3) $n_3^2 = 1,\ \ n_1 = n_2 = 0$ corresponds to θ=0 without restrictions on φ. This is sufficient for the vanishing of the function $N(\varphi,0,\psi)$, thus extreme $\left(2s_{11}-2s_{12}\right)^{-1}$ is impossible.

In special cases, when only one component of the vector **n** vanishes

4) n_1=0, n_2≠0, n_3≠0 corresponds to φ=0. At the same time expression of the vectors **n**, **m** become a simplified form $\mathbf{n}^T = (0,-\sin\theta,\cos\theta)$, $\mathbf{m}^T = (-\sin\psi,\cos\theta\cos\psi,\sin\theta\cos\psi)$. We will have $N(0,\theta,\psi) = \sin^2 2\theta\cos^2\psi = 1$. The last equality can be satisfied only if $\cos^2\psi = 1$ and $\sin^2 2\theta = 1$, and, therefore, if ψ=0,π; θ=π/4,3π/4. As a result:

$N(0,\pi/4,0)$=$N(0,3\pi/4,0)$=$N(0,\pi/4,\pi)$=$N(0,3\pi/4,\pi)$=1.

5) n_2=0, n_1≠0, n_3≠0 corresponds to φ=π/2. Similarly to the previous case, we obtain $\mathbf{n}^T = (\sin\theta,0,\cos\theta)$, $\mathbf{m}^T = (-\sin\psi,\cos\theta\cos\psi,\sin\theta\cos\psi)$ and find exactly the same equation $N(\pi/2,\theta,\psi) = \sin^2 2\theta\cos^2\psi = 1$. It gives the same solutions ψ=0,π; θ=π/4,3π/4. As a result:

$N(\pi/2,\pi/4,0)$=$N(\pi/2,3\pi/4,0)$=$N(\pi/2,\pi/4,\pi)$=$N(\pi/2,3\pi/4,\pi)$=1.

6) n_3=0, n_1≠0, n_2≠0 corresponds to θ=π/2. Here we find $\mathbf{n}^T = (\sin\varphi,-\cos\varphi,0)$, $\mathbf{m}^T = (-\cos\varphi\sin\psi,-\sin\varphi\sin\psi,\cos\psi)$ and $N(\varphi,\pi/2,\psi) = \sin^2 2\varphi\cos^2\psi = 1$. The last equation gives the solutions φ=0,π/2; ψ=0,π. As a result:

$N(0,\pi/2,0)$=$N(0,\pi/2,\pi)$=$N(\pi/2,\pi/2,\pi)$= =$N(\pi/2,\pi/2,0)$=1.

In the more general case

7) n_1≠0, n_2≠0, n_3≠0, because the function N(**n**,**m**)= can be written as

N(**n**,**m**)=1-{$(n_1m_2+n_2m_1)^2$+$(n_1m_3+n_3m_1)^2$+$(n_2m_3+n_3m_2)^2$},

the condition of extremality N(**n**,**m**)=1 is reduced to a system of three linear equations for m_1, m_2, m_3

n_1m_2+n_2m_1 =0, n_1m_3+n_3m_1=0, n_2m_3+n_3m_2=0.

In this case the determinant of this system does not vanish and is equal to D=-2$n_1n_2n_3$. Consequently, the system has not solutions for m_1, m_2, m_3.

5. Summary

Thus, the value of the shear modulus s_{44}^{-1} is maximum in the case P>1 and minimum in case 0<P<1. This extreme is reached in the following sets of Euler's angles (φ,θ,ψ):

at an arbitrary angle φ, θ = π/2 and ψ= 0,

at an arbitrary angle θ, ψ = π/2 and φ =0, π/2,

at an arbitrary angle ψ, θ = π/2 and φ =0, π/2,

at two arbitrary angles φ, ψ and θ =0.

At P>1 value of the shear modulus $\left(2s_{11}-2s_{12}\right)^{-1}$ is minimal, and at 0<P<1 it becomes maximal. This value is reached in the following sets of Euler's angles (φ,θ,ψ): (0,π/4,0), (0,3π/4,0), (0,π/4,π), (0,3π/4,π), (π/2,π/4,0), (π/2,3π/4,0), (π/2,π/4,π), (π/2,3π/4,π), (0,π/2,0), (0,π/2,π), (π/2,π/2,0), (π/2,π/2,π).

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