phys. stat. sol. (b) **207**, 317 (1998)

Subject classification: 61.72.Bb; 61.72.Cc

Gauge Field Theory of Structural Defects and Thermal Tensions

N. M. BOGATOV and H. P. KRYJNIAIA

Department of Theoretical Physics, Kuban State University, 149 Stavropolskaya Str., 350040 Kranodar, Russia

(Received July 16, 1997; in revised form November 13, 1997)

A gauge field theory of structural defects in solid state matter is built. Equations describing structural defects and tension dislocations are obtained. Thermal tensions arising in a ribbon-shaped tape with polysynthetical twin structure grown by EFG method are being considered.

1. Introduction

Changes in temperature processes in different plastic flow regions influence the structure formation of a growing crystal. Because of different conditions the growing structure is not homogeneous and that is why its deformation has rotational and translation components which are described by the gauge field theory.

As is known, there are different gauge field theory versions suggested by different authors. The gauge field theory of dislocations and disclinations using Yang-Mills's idea [1] deals with such problems as defect dynamics, thermodynamcis of solids with defects, elasticity, plastic and strength properties of solids. The solution of field equations for dislocations is introduced in [2]. However, this theory is criticized in [3], where according to the assumption that dislocations and disclinations are translation defects the authors calculate field tensions of defects. The results tend to coincide with classical results for large distances. In [4] the author uses Higges complex fields to describe dislocations and disclinations and draw parallels with quantum electrodynamics. This approach is generalized in [5]. The quantum gauge theory of dislocations is suggested also in [6]. The gauge theory of plastic defects in a medium with a more complicated structure, such as polycrystals is described in [7 to 10]. The gauge group includes a nine-parametrical group of linear transformations of the local basis. Gauge theories using non-Riemann geometry describe only dislocations and disclinations [11]. The gauge theory of dislocations and disclinations in crystals with many-atom gratings is established in [12].

The main aim of this paper is to present a unified approach to the study of the gauge theory of structural defects in solid matter and its comparison with the theory of thermal tensions for areas bounded with crystallization zones.

2. Structural Defect Gauge Theory in an Elastic Continuum

Structural defects are treated as results of the influence of the nonhomogeneous Lee-group of gauge transformations $G = GL(3, R) > T(3)$. This group is a semilinear product of the real nine-parametrical linear transformation group of local basis in solid mat-

ter $GL(3, R)$ [7] on one side and the translational group of spatial variables that characterize point location $T(3)$ on the other. The matrix form of the Lee gauge group is obtained if we inclose the three-dimensional space into a space with more dimensions [1].

An elastic continuum with defects maps on a four-dimension layered space $\mathbf{L}_{4,5}$, which is defined in [13]. A four-dimension Euclidian space R_4 forms a base in $\mathbf{L}_{4,5}$ with the local coordinate system $\bar{e}_\alpha$, $\alpha = 0, 1, 2, 3$, that transfers under coordinate transformations $x^{\alpha'} = x^{\alpha'}(x^\beta)$ according to the law

$$\bar{e}_{\alpha'} = \frac{\partial x^\alpha}{\partial x^{\alpha'}} \bar{e}_\alpha . \tag{1}$$

Space layer $\mathbf{L}_{4,5}$ is a real five-dimensional space of affine coherency L_5 [14] with local basis $\bar{\psi}_{(\alpha)}$, $(\alpha) = 0, 1, 2, 3, 4$ defined in each point of R_4 with coherent object field $\tilde{\mathbf{A}}^{(\mu)}_{\beta(\nu)}$ and metric tensor components defined by the bilinear (scalar in R_4) function $g_{(\alpha)(\beta)} = F(\bar{\psi}_{(\alpha)}, \bar{\psi}_{(\beta)}, x^\gamma)$. The local basis under the point movement from x^β into $x^\beta + \mathrm{d}x^\beta$ transfers as follows:

$$\mathrm{d}\bar{\psi}_{(\nu)} = \tilde{\mathbf{A}}^{(\mu)}_{\beta(\nu)} \bar{\psi}_{(\mu)} \, \mathrm{d}x^\beta . \tag{2}$$

The Lee gauge group G maps into matrix space (5×5) that operates on the local basis,

$$\bar{\psi}_{(\nu')} = M^{-1(\nu)}_{(\nu')} \bar{\psi}_{(\nu)} , \tag{3}$$

$$M_{(0)}{}^{(0)} = M_{(4)}{}^{(4)} = 1, \qquad M_{(4)}{}^{(i)} = b^{(i)} , \qquad M_{(i)}{}^{(0)} = M_{(0)}{}^{(i)} = M_{(4)}{}^{(0)} = M_{(0)}{}^{(4)} = 0 . \tag{4}$$

Under the Lee group elements in the four-dimensional subspace of space L_5 the tensor components $\varphi^{(\alpha)}$ transform as follows:

$$\varphi^{(0')} = \varphi^{(0)} = x^0 , \qquad \varphi^{(i')} = M_{(i)}{}^{(i')} \varphi^{(i)} + b^{(i')} , \qquad \varphi^{(4')} = \varphi^{(4)} = 1 . \tag{5}$$

Here it is assumed that Latin indexes have values 1, 2, 3, Greek without parentheses 0, 1, 2, 3 and Greek with parentheses 0, 1, 2, 3, 4. Time-like components have indexes equal to zero while other values go for space components. The transformation law for the $\tilde{\mathbf{A}}^{(\mu)}_{\beta(\nu)}$ components can be obtained from eqn. (2) and the invariant matrix has the following zero components: $\tilde{\mathbf{A}}^{(4)}_{\beta(\alpha)} = \tilde{\mathbf{A}}^{(0)}_{\beta(\alpha)} = \tilde{\mathbf{A}}^{(\alpha)}_{\beta(0)} = 0$. Let $\tilde{\mathbf{A}}^{(i)}_{\beta(4)} = \theta^{(i)}_\beta$.

The spatial components of the metric tensor could always be transformed using gauge transformations (3), (4) as

$$g_{(i)(j)} = g_{ij} , \tag{6}$$

where g_{ij} are the metric components of the tensor R_4. We consider only spatial structure defects, so therefore

$$g_{(0)(0)} = g_{00} = -1 , \qquad g_{(0)(i)} = g_{0i} = 0 . \tag{7}$$

Equations (6), (7) are true in the local basis $\bar{\psi}_{(\alpha)}$ of space L_5. We will call it a picked basis because it depends upon the choice of the coordinate system in R_4 space.

Field variables $\varphi^{(i)}$, $\tilde{\mathbf{A}}^{(i)}_{\beta(j)}$, $\theta^{(i)}_\beta$ describe the elastic continuum with defects. Distortion tensor components can be used to describe the field changes $\varphi^{(i)}$ under the local basis

$$B_{(\beta)}{}^{(i)} = \nabla_\beta \varphi^{(i)} = \frac{\partial}{\partial x^\beta} \varphi^{(i)} + \tilde{\mathbf{A}}^{(i)}_{\beta(j)} \varphi^{(j)} + \theta_\beta{}^{(i)} , \qquad B_\beta{}^{(0)} = \delta_\beta{}^0 , \qquad B_\beta{}^{(4)} = 0 , \tag{8}$$

where ∇_β denotes the covariant derivative in L_5. According to the definition given in [15] the deformation tensor is

$$u_{\alpha\beta} = \tfrac{1}{2}\,(g_{(\mu)(\nu)}B_\alpha{}^{(\mu)}B_\beta{}^{(\nu)} - g_{\alpha\beta})\,. \tag{9}$$

Let us pick the Lagrangian density of the elastic continuum with defects as

$$L = (L_0 + s_1L_1 + s_2L_2)\,\sqrt{|g|}\,, \tag{10}$$

$$L_0 = C^{\beta\gamma\mu\nu}(u_{\beta\gamma} - \alpha_{\beta\gamma}T)\,(u_{\mu\nu} - \alpha_{\mu\nu}T)/2\,, \tag{11}$$

$$L_1 = g^{\mu\nu}g^{\beta\gamma}(3\mathbf{R}^{(i)}_{\mu\beta,\,(j)}\mathbf{R}^{(j)}_{\nu\gamma,\,(i)} - \mathbf{R}^{(i)}_{\mu\beta,\,(i)}\mathbf{R}^{(j)}_{\nu\gamma,\,(j)})\,, \tag{12}$$

$$L_2 = -g^{\mu\nu}g^{\gamma\delta}g_{(i)(j)}(\nabla_\gamma B_\mu{}^{(i)} - \nabla_\mu B_\gamma{}^{(i)})\,(\nabla_\delta B_\nu{}^{(j)} - \nabla_\nu B_\delta{}^{(j)})/2\,, \tag{13}$$

where $C^{ijkh} = -c^{ijkh}$, c^{ijkh} are the crystal elastic rigidity coefficients; $C^{0h0k} = \varrho g^{hk}$, ϱ is the material density; $C^{0\alpha ij} = C^{000\delta} = C^{00\alpha\beta} = 0$; $C^{\beta\gamma\mu\nu} = C^{\gamma\beta\mu\nu} = C^{\beta\gamma\nu\mu} = C^{\mu\nu\beta\gamma}$; α_{ij} is the crystal heat expansion tensor, $\alpha_{\sigma j} = 0$; ∇_γ is the operator which denotes the covariant derivative with the coherence coefficients $\tilde{A}^i_{\gamma j} = g^{ik}(\partial_\gamma g_{kj} + \partial_j g_{\gamma k} - \partial_k g_{\gamma j})/2$ for indexes without parentheses and $\tilde{A}^{(i)}_{\gamma(j)} = \tilde{A}^i_{\gamma j}$ (in the picked local basis) for indexes in parentheses;

$$\mathbf{R}^{(\alpha)}_{\mu\gamma,\,(\beta)} = \frac{\partial}{\partial x^\gamma}\,\tilde{\mathbf{A}}^{(\alpha)}_{\mu(\beta)} - \frac{\partial}{\partial x^\mu}\,\tilde{\mathbf{A}}^{(\alpha)}_{\gamma(\beta)} + \tilde{\mathbf{A}}^{(\alpha)}_{\gamma(\xi)}\tilde{\mathbf{A}}^{(\xi)}_{\mu(\beta)} - \tilde{\mathbf{A}}^{(\alpha)}_{\mu(\xi)}\tilde{\mathbf{A}}^{(\xi)}_{\gamma(\beta)} \tag{14}$$

the curvature tensor in the affine coherent space L_5.

The Lagrangian density (10) to (13) includes values that have the following physical interpretation:

$\sigma^{ij} = -C^{ijkh}(u_{kh} - \alpha_{kh}T)$ are the stress tensor components, $\sigma^{0h} = 2C^{0h0k}u_{0k}$ is the impulse density of a material medium, $P^{\mu\nu(\alpha)} = \text{sign}\,(g)\,\varepsilon^{\mu\nu\beta\gamma}\mathbf{R}^{(\alpha)}_{\alpha\beta,\,(\xi)}\varphi^{(\xi)}/2$ is the dislocation density tensor, $D^{\mu\nu(\alpha)}_{(\delta)} = \text{sign}\,(g)\,\varepsilon^{\mu\nu\beta\gamma}\mathbf{R}^{(\alpha)}_{\mu\beta,\,(\delta)}/2$ is the disclination density tensor, $\varepsilon^{\mu\nu\beta\gamma}$ is the Levi-Civita completely antisymmetric tensor.

Using the Lagrangian density from (10) to (13) we can get the field equations

$$\nabla_\eta X^\eta{}_{(h)} = 0\,, \qquad \nabla_\eta Z^{\lambda\eta}{}_{(h)} - X^\lambda{}_{(h)} = 0\,, \qquad D_\eta U^{\lambda\eta(f)}{}_{(h)} = 0\,, \tag{15}$$

where D_η is the covariant derivative operator with coherent coefficients as follows:

$$\tilde{\mathbf{A}}^{(\alpha)}_{\mu(\beta)}\,, \quad \tilde{\mathbf{A}}^{\alpha}_{\mu\beta}; \quad X^\eta_{(h)} = \sigma^{\mu\eta}g_{(\alpha)(h)}B_\mu{}^{(a)}\,; \quad Z^{\lambda\eta}_{(h)} = s_2 2g^{\lambda\mu}g^{\eta\gamma}g_{(h)(j)}(\nabla_\gamma B_\mu{}^{(j)} - \nabla_\mu B_\gamma{}^{(j)})\,;$$

$$U^{\lambda\eta(f)}{}_{(h)} = s_1 4g^{\lambda\mu}g^{\eta\gamma}(3\mathbf{R}^{(f)}_{\mu\lambda,\,(h)} - \delta_{(h)}{}^{(f)}\mathbf{R}^{(i)}_{\mu\gamma,\,(j)})\,.$$

In case of small deformations $B_\mu{}^{(\xi)} \approx \delta_\mu{}^{(\xi)}$ with $\varphi^{(\xi)} = x^\xi + u^{(\xi)}$ from eqn. (15) we can derive the equilibrium equation $\nabla_\mu\sigma^{\nu\mu} = 0$ and in case $\tilde{A}^{(i)}_{\beta(j)} = 0$ we get field equations described in [3].

2.1 Structure building during the silicon ribbon growth by the EFG method

Parallel microtwins made out of polycrystal silicon grown by the EFG method have some advantages when used in the production of sun elements [16]. Average tangent thermal tensions in the polysynthetical region do not reach critical values that cause dislocation formation [17]. Let us analyze the opportunity of getting ribbons with low dislocation densities using the above-discussed gauge theory.

Using eqn. (9) and (15) in case of a stationary growth regime and insignificant deformations, we get the following equation:

$$S_{bkpt}\,\Delta\sigma^{pt} + S^{i}{}_{ipt}(\nabla_b\nabla_k - \tfrac{1}{2}\,g_{bk}\Delta)\,\sigma^{pt} - S^{i}{}_{kpt}\nabla_i\nabla_b\sigma^{pt} - S^{i}{}_{bpt}\nabla_i\nabla_k\sigma^{pt} + \tfrac{1}{2}\,g_{bk}S^{rj}{}_{pt}\nabla_r\nabla_j\sigma^{pt} + \nabla_b\nabla_k\alpha T - \tfrac{1}{2}\,s_2(\sigma_{bk} - \tfrac{1}{2}\,g_{bk}\sigma^{i}{}_{i} - \tfrac{1}{2}\,g^{i(l)} \times (\nabla_b Z_{ki(l)} + \nabla_k Z_{bi(l)})) = 0\,, \tag{16}$$

where S_{bkpt} are the crystal compliance coefficients; Δ is the Laplacian operator, $\alpha_{ij} = g_{ij}\alpha$, $g^{i(l)} = g^{il}$. Equation (16) transforms into a usual thermal tension equation under the condition $s_2 \to \infty$.

We assume that the crystallographic surface orientation of the ribbon is (110), direction of growth $[1\bar{1}2]$ opposite to the temperature gradient. Twin borders Σ_3 have orientation $(\bar{1}11)$ and are W_l apart. The orientation of the local coordinate system in R_4 space is $\vec{e}_1 = 1/\sqrt{2}$ [110], $\vec{e}_2 = 1/\sqrt{3}$ $[\bar{1}10]$, $\vec{e}_3 = 1/\sqrt{6}$ $[1\bar{1}2]$. Such twins are rotation twins and that is why

$$\vec{\Psi}_{(r)} = K^{i}{}_{(r)}\vec{e}_i\,, \qquad K^{1}{}_{(2)} = -K^{2}{}_{(1)} = \sin\varphi\,, \qquad K^{1}{}_{(1)} = -K^{2}{}_{(2)} = \cos\varphi\,,$$
$$K^{3}{}_{(1)} = K^{3}{}_{(2)} = K^{1}{}_{(3)} = K^{2}{}_{(3)} = 0\,, \qquad K^{3}{}_{(3)} = 1\,.$$

For Σ_3 border with $y = y_c$ location $\varphi(y) = -\pi\theta(-(y - y_c))$. From eqn. (2) we can find non-zero components $\tilde{\mathbf{A}}^{(1)}_{2(2)} = -\tilde{\mathbf{A}}^{(2)}_{2(1)} = \Sigma_c\pi\delta(y - y_c)$. Transferring to new variables $\theta^{(s)}_{\beta} = f^{(s)}_{\beta} - \tilde{\mathbf{A}}^{(s)}_{\beta(r)}\varphi^{(r)}$ we will get dislocation density tensor as

$$P^{0j(h)} = e^{jki}\left[\frac{\partial}{\partial x^i}\,f_k{}^{(h)} + \tilde{\mathbf{A}}^{(h)}_{i(l)}\delta_k{}^{(l)} + \tilde{\mathbf{A}}^{(h)}_{i(l)}\left(f_k{}^{(l)} + \frac{\partial}{\partial x^k}\,u^{(l)}\right)\right], \tag{17}$$

where e^{jki} equals unity if index permutation is even and -1 if it is odd. The second item in the brackets of eqn. (17) characterizes twin borders, the third and fourth ones defect generation on those borders. The following boundary conditions are true for ideal borders Σ_3:

$$f_1{}^{(2)} = f_{(3)}{}^{(2)} = f_1{}^{(1)} = f_3{}^{(1)} = 0\,, \qquad \frac{\partial}{\partial x^1}\,u^{(2)} = \frac{\partial}{\partial x^3}\,u^{(2)} = \frac{\partial}{\partial x^1}\,u^{(1)} = \frac{\partial}{\partial x^3}\,u^{(1)} = 0\,.$$

Using gauge conditions [1] $\nabla_i f^{i(h)} = 0$, $f^{k(h)} = f^{h(k)} = f^{kh}$, we get

$$\Delta f^{kh} = \frac{\sigma^{kh}}{2s_2}\,, \qquad Z^{(h)}_{ki} = 2s_2\left(\frac{\partial}{\partial x^i}\,f_k{}^{(h)} - \frac{\partial}{\partial x^k}\,f_i^{(h)}\right). \tag{18}$$

The coefficients $\tilde{\mathbf{A}}^{(\alpha)}_{\mu(\beta)}$ satisfying the field equations can be obtained. Substituting (18) into (16) we get an equation for f^{kh}. From (18) we derive σ^{kh}. The approximate solution for a thin plane ribbon with low density is

$$f^{23} = A(y - y_l)\,(7 - 40Y^2 + 48Y^4)\,T'''(z)\,, \tag{19}$$

$$f^{33} = -A(7 - 120Y^2 + 240Y^4)\,T''(z)\,, \tag{20}$$

$$f^{22} = -A[(\tfrac{7}{2} - 10Y^2 + 8Y^4)\,(y - y_l)^2\,T''''(z) + 8T''(z)]\,, \tag{21}$$

where $A = (\alpha E W_l^4)/(s_2 \cdot 1.152 \times 10^4)$; $Y = (y - y_l)/W_l$, $y \in [y_l - W_l/2,\ y_l + W_l/2]$; y_l is the twin-block center coordinate. Expressions obtained for σ^{33}, σ^{23}, σ^{22} are identical to

those found in [17]. $E = 2.52 \times 10^7$ N cm^{-2}, and is larger than Young's modulus $E = S_{11}^{-1} = 1.3 \times 10^7$ N cm^{-2}.

Let us find tangent tensions in the main system of sliding planes and decompose the dislocation density tensor (17) into system elements. The maximum tangent tension value τ which arises in the neighborhood of the twin borders is

$$\tau = |\tau_{[0\bar{1}1](111)}|_{\max} = \frac{\alpha E W_l^2 T''}{12\sqrt{6}} . \tag{22}$$

3. Conclusion

The formation of twinning borders, occurring in the plastic flow region during crystal growth, was explained by means of the gauge field theory using geometrical reasoning.

Dislocations develop under thermal tensions for the case $\tau > \tau_{\text{critical}}$. Near the crystallization front at temperature $T_0 \approx 1688$ K the critical tension value for dislocation formation in Si is $\tau_{\text{critical}} = (5 \text{ to } 10) \times 10^{-3}$ N cm^{-2} [18]. In the observed technological process $T'' \approx 10^3$ K cm^{-2}. Taking $\alpha = 4.15 \times 10^{-6}$ K^{-1} and substituting eqn. (22) into the condition $\tau < \tau_{\text{critical}}$, we will get $W_l < 0.12$ cm. According to [16] the twin border distance in the Si ribbon is not greater than 0.1 cm. Hence, the twinning effect is responsible for thermal tension fall.

The obtained approximate solution is true if $EW_{l\max}^2/48s_2 \ll 1$. Thus, we get thermoelastic theory transfer conditions: $s_2 \gg 5.25 \times 10^3$ N. In this case for the main system sliding plane elements dislocation boundary densities have small values that is $N_{\max} \ll 10^3$ cm^{-2}.

References

[1] A. Kadic and D. Edelen, A Gauge Theory of Dislocations and Disclinations, Izd. Zinatne, Moscow 1987.
[2] V. A. Osipov, Phys. Lett. A **146**, 67 (1990).
[3] M. C. Valsakumar and D. Sahoo, Bull. Mater. Sci. **10**, 3 (1988).
[4] H. Kleinrert, J. Phys. A **19**, 1855 (1986).
[5] H. Kleinert, Gauge Fields in Condensed Matter, Vol. 2, Stresses and Defects, World Scientific Publ. Co., Singapore 1989.
[6] A. I. Musienko, Physical Thought of Russia No. 3, 3 (1996).
[7] V. E. Panin, U. V. Grinyaev, V. E. Egorushkin, I. L. Bukhbinder, and S. N. Kulkov, Izv. vuzov, Fiz. **30**, 34 (1987).
[8] V. E. Panin, Izv. vuzov, Fiz. **33**, 4 (1990).
[9] V. E. Egorushkin, Izv. vuzov, Fiz. **33**, 51 (1990).
[10] V. E. Panin, Izv. vuzov, Fiz. **35**, 5 (1992).
[11] Y. S. Duan and Z. P. Duan, Internat. J. Engng. Sci. **24**, 513 (1986).
[12] A. I. Musienko and V. A. Kopcik, Kristallografiya **41**, 586 (1996).
[13] N. P. Konoplieva and V. N. Popov, Gauge Fields, Izd. Atomizdat, Moscow 1980 (in Russian).
[14] P. K. Rashevski, Riemannian Geometry and Tensor Analysis, Izd. Nauka, Moscow 1967 (in Russian).
[15] L. I. Sedov, Mechanics of Continuous Medium, Vol. 1, Izd. Nauka, Moscow 1976.
[16] M. P. Matveyakin, T. A. Ovchinikova, and V. V. Kasatkin, All Union Conf. Problems of Obtaining Profiled Crystals and Products Using Stepanovs Method and Their Usage in Industry, March 16 to 18, 1989, Leningrad (pp. 188 to 192).
[17] N. M. Bogatov, ibid. (pp. 193 to 198).
[18] M. G. Milvidskii and V. B. Osvenskii, Problems of Modern Crystallography, Izd. Nauka, Moscow 1975 (pp. 79 to 109).