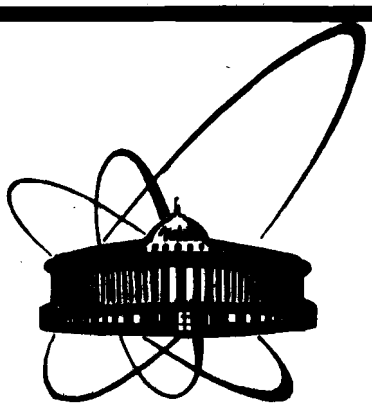

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SIMULATION OF PLASTIC DEFORMATION IN BCC POLYCRYSTALS WITH THE TAYLOR THEORY

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Introduction

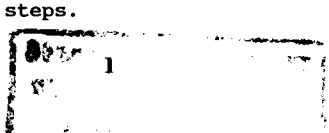
The most of technically important materials are based on crystals. Therefore, crystalline parameters and their anisotropy determine the macroscopic properties of materials in a high degree. Besides classical characteristics of the crystalline phases such as crystal symmetry, chemical composition, shapes and sizes of grains, etc., the orientation distribution of the crystallites becomes more and more interesting. In materials manufacturing deformations of different types are very important technological steps. Consequently one of the main field for texture investigation is the description of plastic deformation processes. Corresponding experimental studies have been carried out for a long time (see the monograph Wassermann-Greven /1/). Fundamental theoretical works become possible since powerful computers have been available. Some models for simulation of plastic deformation of polycrystalline ensembles have been developed and tested in the last years /2/,/3/,/4/. Those models which yield the best agreement with experimental results are based on the Taylor model /5/. Some improvements were introduced by van Houtte /6/. Especially cold deformation textures of fcc metals were predicted in some works with these models till now. Other crystal systems like bcc or hcp have been considered in a less extended manner. In the present work we summarize the essential ideas of the theory of Taylor and their use for modeling plastic deformation and their application to rolling deformation of bcc metals.

Taylor Model

The Taylor model is based upon two main assumptions :

- each grain undergoes the same strain as the whole sample
- this strain is supposed to be realized by multiple slip on different slip systems

These statements correspond to the experimentally observed plastical behaviour of polycrystals, especially with the material continuity at grain boundaries and with the actuation of multiple slip systems in case of higher deformation steps.



For mathematical treatment it is necessary to introduce sample fixed and crystal fixed coordinate systems (see Fig.1). The sample fixed or external system K_A is an orthogonal system (x_1,x_2,x_3) well adapted to the sample and deformation geometry. The crystal fixed system K_B is adapted to the crystallite, in the case of cubic structure we have an orthonormal system (x_1^c,x_2^c,x_3^c). Usually the orientation of the crystal fixed system with respect to the sample fixed system will be described by the direction cosines of its axes with the help of the so-called orientation matrix G (an orthogonal 3x3 matrix) or by the three Euler angles φ_1,ϕ,φ_2 as used by Bunge et al /7/.

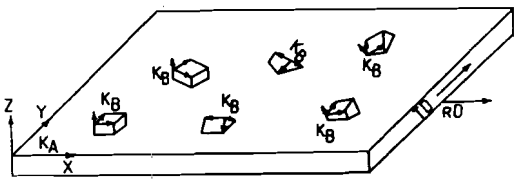


Fig. 1. The sample fixed coordinate system K_A and the crystal fixed coordinate system K_B.

The macroscopic strain tensor **E** is known in the sample system, but the simulation must be carried out for every individual crystallite. The microscopic strain tensor $\mathbf{E}^c$ could be calculated from **E** by :

$$\mathbf{E}^c = G\,\mathbf{E}\,G^T \qquad (1)$$

$\mathbf{E}^c$ can be split up in a symmetric and in a asymmetric part as follows:

$$\mathbf{E}^c = \mathbf{E}_s^c + \mathbf{E}_a^c \qquad (2)$$

$$\mathbf{E}_s^c = (\mathbf{E}^c + \mathbf{E}^{cT})/2 \qquad \mathbf{E}_a^c = (\mathbf{E}^c - \mathbf{E}^{cT})/2\ ,$$

where the symmetric component $\mathbf{E}_s^c$ represents a change in shape, and the antisymmetric component $\mathbf{E}_a^c$ represents a rotation of the selected crystallite. On the other hand, crystallographic shear δ^i in the slip system i gives a change in shape

$$\mathbf{E}_{s\ slip}^{ci} = \delta^i\,\mathbf{s}^i \qquad (3)$$

$$S_{kl}^i = (r_k^i\,v_l^i + r_l^i\,v_k^i)/2$$

r_1^i, r_2^i, r_3^i - direction cosines of slip direction to K_B

v_1^i, v_2^i, v_3^i - direction cosines of normal on slip plane to K_B

and a rotation

$$\mathbf{E}_{a\ slip}^{ci} = \delta^i\,\mathbf{R}^i \qquad (4)$$

$$R_{kl}^i = (r_k^i\,v_l^i - r_l^i\,v_k^i)/2\ .$$

Plastic deformation in a crystallite can be realized by activating of 5 independent slip systems (von Mises /8/) that means summation must be carried out over 5 slip systems. Summation over all activated slip systems produces for the selected crystallite resulting deformation and rotation

$$E_{s\ slip\ kl}^c = \sum_{i=1}^{5} \delta^i\,S_{kl}^i \qquad , \qquad E_{a\ slip\ kl}^c = \sum_{i=1}^{5} \delta^i\,R_{kl}^i\ . \qquad (5)$$

From the first Taylor assumption, strain equality, follows :

$$\mathbf{E}_s^c = \mathbf{E}_{s\ slip}^c \qquad (6)$$

$$\mathbf{E}_a^c = \mathbf{E}_{a\ slip}^c + \mathbf{E}_{a\Delta}^c\ . \qquad (7)$$

The rotation $\mathbf{E}_{a\Delta}^c$ must be added because in general no correspondence between macroscopic rotation of the sample and rotation of the crystallit due to shear can be expected (see Fig.2). This additional rotation $\mathbf{E}_{a\Delta}^c$ determines the orientation change of the selected crystallite (the texture development) by plastic deformation. For calculation of $\mathbf{E}_{a\Delta}^c$ the unknown shear δ^i will be determined from (6), (7) suppling the additional rotation; $\mathbf{E}_s^c$ and $\mathbf{E}_a^c$ can be considered as known. The solution of (6) is not unique, there exists a high degree of freedom in choice of a concrete solution (e.g. using the 3 typical slip systems of bcc crystal class there are 1 712 304 possible variants for different shear, all fulfilling the Taylor assumptions). To overcome this, Taylor introduced the condition, that the solution to be selected is the one that minimizes the internal work during plastic deformation $W^c = \sum_{i=1}^{m} \tau^{ci}\,|\gamma^i|$

τ^{ci} - critical resolved shear stress.

Now (6) and (7) can be effectively dealt with the formalism of linear optimization, mostly with the SIMPLEX algorithm. Unfortunately, in contrast to classical problems of linear optimization the optimal solutions are not unique because of the high symmetry of the problem. This is a serious complication, since for description of plastic deformation processes all possible solutions must be calculated and considered. There exist different ways to calculate the lattice rotation $\mathbf{E}_{a\Delta}^c$ from the multiple solutions. Usually Monte Carlo methods, averaging or additional physical restrictions (e.g. latent hardening of activated slip systems, relaxation of geometrical constraintments) were used.

For simulation a plastic deformation the above discussed formalism must be carried out for a statistical representative number of crystallites respective for a certain number of small deformation steps.

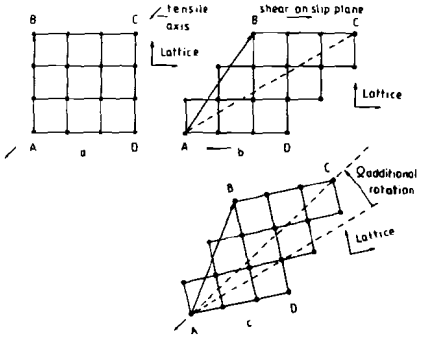


Fig. 2. a,b - A shear δ on a slip plane does not rotate the lattice, although a material vector may be rotated(vector AB e.g.)

b,c - An additional rotation - which is also executed by the crystal lattice - will bring the crystal in a position corresponding with the imposed strain; e.g. pure elongation in the direction AC /6/.

The new crystallite orientations found after a deformation step are the start orientations for the next step. The initial orientation set could be chosen randomly or specially so that an orientation distribution near the isotropic one is represented.

Inverse Pole Figures for Representation of Orientation Distributions

Inverse pole figures represent in a stereographic projection the orientation distribution of an external sample axis within the crystal coordinate system /7/. From this special projection is seen which orientations of the polycrystal are parallel to a given direction of the sample (mostly to the normal direction).

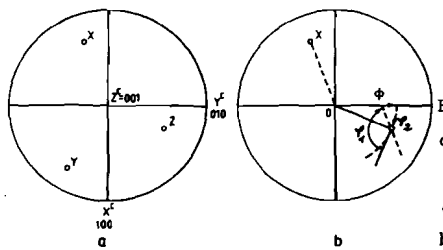


Fig. 3. Representation of a crystal orientation in inverse pole figures
a) Representation of sample-fixed axis in the crystal-fixed frame,
b) Convention used by P. van Houtte.

To increase the evidence of inverse pole figures we use the extended representation of van Houtte (Fig. 3)/6/. Instead of plotting the sample axes x_1, x_2, x_3 in the standard projection of the crystal only the x_3-axis with a special symbol will be plotted. The center of the small circle represents the projection of the x_3-axis, the small stroke is directed parallel to the direction $0X_1$.

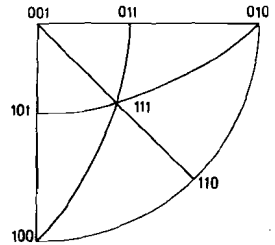


Fig. 4. General fundamental area in orientation space for cubic crystals.

Resulting from the cubic crystal symmetry it is sufficient to consider only a fundamental area of the inverse pole figure (in Fig.4 the two projected spherical triangles 001-011-111 and 001-101-111). Any possible orientation outside this range can be transformed by symmetric transformations into the fundamental area. Taking advantage from the deformation symmetry we can in most cases further reduce the fundamental area to the triangle 001-011-111.

Results of Simulation

Starting from a quasi isotropic initial orientation distribution, represented by a set of 147 single orientations, the Taylor simulations were computed. The parameters were chosen to simulate a plain strain deformation of a bcc metal. 40 single deformation steps, each realizing 5 % reduction, were applied to a total deformation of 87 %. The non-uniqueness of the optimal solutions was considered in all calculations by averaging.

Fig. 5 shows the stepwise texture development, calculated for the main slip system {110}<111>. Clearly seen is a homogeneous 'flowing' of the single orientations to the final components. By more detailed interpretation of the final distribution we can point out final directions in the orientation tube {112}<9 $\overline{11}$ 1> to {344}<4$\overline{5}$2>. With the help of the simulation method we studied the effect of the experimentally determined slip systems {110}<111>, {112}<111> and {123}<111> to the resulting final texture independently of each other or in any correlation. The respective final orientations are shown in Fig. 6. Although

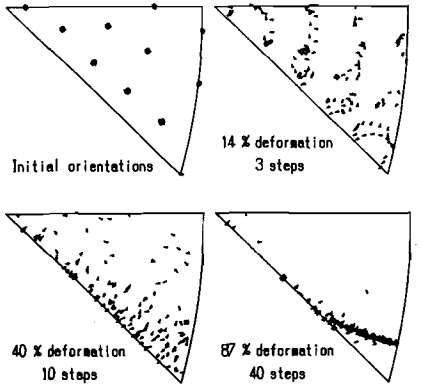


Fig. 5. Texture development of plain strain deformation of bcc crystals calculated by simulation of multiple slip on {110}<111> slip systems. The 147 crystallite orientations were initially equally distributed over the fundamental area 001-011-111.

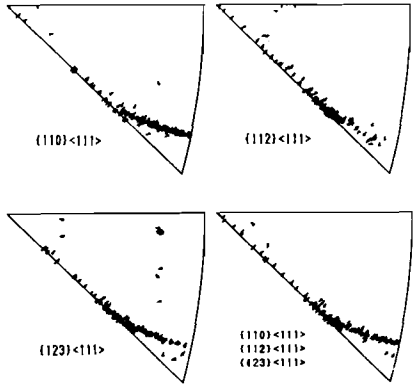


Fig. 6. Final textures of simulated plain strain deformations of bcc crystals, different active slip systems were used in the simulation.

the individual influence of the different slip systems is seen, a general tendency is established. From the simulation analysis follows:

slip system	final rolling texture
{110}<111>	(112)[$9\bar{1}\bar{1}$1] to (344)[$4\bar{5}2$]
{112}<111>	(5511)[$11\bar{0}$] to (335)[$11\bar{0}$]
{123}<111>	(337)[$1\bar{1}0$] to (456)[$54\bar{0}$] + (1811)[$01\bar{1}\bar{8}$]
({110}+{112}+{123})<111>	(5511)[$1\bar{1}0$] to (344)[$\bar{4}52$]

This represents a correspondence to measured rolling textures of bcc metals. There were found texture components at orientations:

α-fibre ([110] parallel to the rolling direction)
from (001)<$1\bar{1}0$> to (111)[$1\bar{1}0$]
β-fibre
from (112)<$11\bar{0}$> to (11 8 11)[4 11 4]
γ-fibre ((111) parallel to the rolling plane)
from (111)<$11\bar{0}$> to (111)[$12\bar{0}$]

These rolling textures may vary strongly from one bcc metal to another, and even materials with identical chemical compound differ in their deformation character from each other. The existing deviations of the simulation to the experimental results are interpreted as a not complete adapting of our model to the deformation process and as specific influence of experimental conditions such as inhomogeneous deformation and start texture.
Comparing the simulation results and the above given experimental behaviour of bcc metals it is seen, that with the used general conditions for describing plane strain a good agreement for development of β-fibre and somewhat less good for γ-fibre is possible. The simulation does not supply positions (001) parallel to the rolling plane and also the exact position of (111) parallel to the rolling plane is not supported.

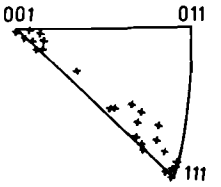


Fig. 7. Experimental inverse pole figure of a cold rolled Fe Si-sheet (82% deformation)

For comparison with experimental results Fig.7 shows the inverse pole figure of a Fe-3 w% Si-sheet, that has been rolled at room temperature, the rolling reduction was 82 % /9/. The texture development of polycrystalline samples was there investigated by stepwise rolling and careful measuring of the orientations of specially selected single crystals. The final deformation state of the 37 representative crystals shows that our simulation is in agreement with the real texture. The components near (001) parallel to the rolling direction are missing in the modeling.

To overcome the existing disagreements further simulations should be calculated by including individual parameters with respect to the chosen materials (e.g. special weightening of activated slip systems, relaxing of geometrical constraintments especially at higher deformation steps and consideration of actual start orientation distribution).

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Моделирование пластичной деформации
в объемно центрированных кубических
поликристаллах на основе теории Тайлора

В данной работе изложены основы модели Тайлора. Эта модель самая распространенная для моделирования развития текстур на базе таких микроскопических процессов, как скольжение. Результаты расчетов для разных степеней деформации ОЦК-поликристаллов сравниваются с экспериментальными данными.

Работа выполнена в Лаборатории нейтронной физики ОИЯИ.

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Simulation of Plastic Deformation
in BCC Polycrystals with the Taylor Theory

In this paper the essential ideas of the Taylor theory are summarized. This Taylor model is the most used model to understand the development of texture on the base of microscopic processes like slip or glid. Calculations for various degrees of deformations were done for BCC materials.

The investigation has been performed at the Laboratory of Neutron Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1989