Crystal Plasticity Simulation of Hot Deformation Texture of Titanium Alloy Considering Alpha-beta Transformation

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Abstract. Titanium alloys are usually subjected to hot deformation to optimize its microstructure and mechanical property. In the hot forming process, such as extrusion, texture is of great importance to both manufacturing and performance. In this study, an alpha-beta titanium was used to study the texture evolution during hot extrusion. Large area electronic backscattering scan was used to examine grain orientation distribution. Experimentally measured alpha and beta textures were compared with a rate-dependent crystal plasticity based simulation. The model is capable of predicting the deformation textures of both alpha and beta phases at extrusion temperature. The model also takes into account the transformation of metastable beta phase to alpha phase in the cooling process, considering variant selection. The transformation texture components mostly have [0001] along extrusion direction, forming the primary component of alpha extruded texture. The model works well in predicting hot deformation texture of titanium alloy.

1. Introduction
Titanium alloys, with lightweight and excellent mechanical properties, have been widely used in aeronautic industry, marine ships, nuclear components, medical instruments, and so on [1]. Alpha-beta titanium alloy has excellent elevated strength, formability, and corrosive resistance, is becoming an important material in future nuclear industry. For titanium alloy with alpha and beta phases, it is sensitive to hot deformation process, which affects dramatically the microstructure, such as grain/colony size, lamellar spacing, and texture. Apparently, it further determines the mechanical property of alloy. Hence, both industry and academia realize that it is crucial to have computational tools for predicting the interrelationship between processing, microstructure, and property. In the United States, both the Materials Genome Initiative and Integrated Computational Materials Engineering (ICME) community have been making efforts to develop methodology integrating the resources of theory, simulation and experiments.

For titanium alloys with low crystal symmetry of hcp structure, hot extrusion are used as a typical processing, typically in the α+β temperature field where there is higher fraction of β phase than that at room temperature. During the post-cooling process after hot deformation, the metastable β phase will partially decomposes into α phase, following the well-known Burgers orientation relationship (BOR), i.e. (0001)(110) and [-2110][11-1]. Hence, to predict the microstructure evolution during hot
processing, the $\beta \rightarrow \alpha$ transformation must be taken into account. For hot extrusion of titanium alloy, the final texture should consider three important aspects: (i) $\alpha$ deformation texture at the forming temperature, (ii) $\beta$ deformation texture at the forming temperature, and (iii) $\alpha$ transformation texture formed during the $\beta \rightarrow \alpha$ transformation, in which there are 12 possible variants according to the crystal symmetry of $\alpha$ and $\beta$ phase. Usually, bias selection of certain $\alpha$ variants would occur, which will affect the transformation $\alpha$ texture.

For a computational toolset for predicting the hot texture of titanium alloy, crystal plasticity based models have been widely used in previous studies, as they can capture the plastic deformation mechanisms of slip. For modeling the texture evolution during large deformation of polycrystalline materials, approaches in literature include classical Taylor models [2,3], relaxed-constraint (RC) Taylor model [4], multiple grain models [5], viscoplastic self-consistent (VPSC) model [6,7], and crystal plasticity finite element (CPFE) methods [8-11]. The CPFE approach is quite promising in capturing microstructural effects, however it requires significant computational resources to model an industrial extrusion process. There have been some efforts to reduce computational cost, it is increasingly accepted nowadays to use uncoupled continuum FEM and crystal-plasticity model for simulating extrusion or forging process [12]. For instance, Glavivic et al. [13] modeled the forging process of Ti6Al4V and location-specific texture distribution in the forged pancake, by using commercial finite element software to analyze crystal orientation due to metal flow and Taylor-type polycrystalline plasticity codes to calculate the rotation due to crystal plasticity.

This paper reports a crystal plasticity model based toolset for hot texture of titanium alloy. The toolset can be used to predict the “processing-microstructure”, i.e. simulating the texture evolution during and subsequent to the hot extrusion of $\alpha+\beta$ titanium alloy, taking into account $\beta \rightarrow \alpha$ transformation process [14]. The validity of this computationally efficient, sequential simulation approach has been validated by successfully reproducing the experimental $\alpha$ extrusion texture.

2. Materials and Experimental

In this study, an $\alpha+\beta$ titanium alloy was used. It has a high volume fraction of primary $\alpha$ grains, i.e. 70-90% (grain size of ~5 µm). Fig. 1 is the (0001) pole figure obtained from EBSD, indicating slight texture (with an intensity of ~4x random on average) in the as-received state. The extrusion was conducted at 900°C at an extrusion ratio of 14. The extruded bar was sectioned along the longitudinal section, grinded and polished. Large area EBSD scan was conducted to obtain the grain orientation information. Fig. 1 shows the pole figure from EBSD after extrusion. It is seen that the 0001 poles are preferentially aligned along the extrusion direction.

![Figure 1. Alpha texture of extruded titanium alloy indicated by EBSD IPF (“ED” is outwards)](image)

3. Crystal Plasticity Theory and Finite Element Simulation

3.1. Crystal Plasticity Theory

For the texture prediction, a rate dependent crystal plasticity model is used, based on the classical crystal plasticity theory developed by Hill [15], Asaro and Rice [16]. The deformation of a crystalline
material under external load consists of elastic deformation and inelastic deformation. The total deformation gradient \( F \) can be separated into elastic and plastic part and given by

\[
F = F^e \cdot F^p, \quad \det \left( F^p \right) = 1, \quad \det \left( F^e \right) > 1. \quad (1)
\]

Where \( F^e \) denotes the part of elastic deformation, \( F^p \) denotes the part of plastic deformation. The rate of change of \( F^p \) is related to shearing rate \( \dot{\gamma}^{(a)} \) of \( \alpha \) slip system as follow:

\[
\dot{F}^p \cdot F^{p-1} = \sum_{\alpha} \dot{\gamma}^{(a)} s^{(a)} m^{(a)} \quad (2)
\]

where \( \dot{\gamma}^{(a)} \) is the resolved shear strain rate on \( \alpha \) slip system, \( m^{(a)} \) is the slip normal direction on \( \alpha \) slip system, \( s^{(a)} \) is the slip direction on \( \alpha \) slip system.

The resolved shear stress \( \tau^{(a)} \) on each slip system is obtained via the Schmid’s law. The shearing rate \( \dot{\gamma}^{(a)} \) of \( \alpha \) slip system is expressed by the resolved shear stress \( \tau^{(a)} \), given by:

\[
\dot{\gamma}^{(a)} = \gamma_0 \left[ \frac{\tau^{(a)}}{g^{(a)}} \right]^{1/m} \quad (when \ \tau^{(a)} > g^{(a)}) \quad (3)
\]

where \( \gamma_0 \) and \( \tau^{(a)} \) are the shear strain rate and resolved shear stress on slip system \( \alpha \) respectively, \( g^{(a)} \) is the reference shearing rate, \( g^{(a)} \) is the slip resistance on slip system \( \alpha \), \( m \) is the rate sensitivity exponent [17-18].

3.2. Finite Element Model

For computing the hot extrusion texture, finite element simulation of the extrusion process was firstly conducted. The actual dimensions of extrusion die and billet, extrusion rate etc was used in the simulation. The stress and strain values along the central axis of billet were obtained from the stress and strain contour. At the billet central axis, the deformation of alpha and beta phase can be regarded as bi-axial compression along x and y axis, perpendicular to the extrusion direction (z axis). The strain values were used as boundary condition for crystal plasticity finite element model in Fig. 2, in which 1024 C3D8R elements were used. Each element represents a grain. The deformation texture of alpha and beta phase can be obtained from crystal plasticity simulation of finite element model in Fig. 2.

![Figure 2. Finite element model for predicting the extrusion texture near extrusion billet central axis](image-url)
4. Results and Discussion
Crystal plasticity finite element simulation of titanium hot extrusion with ratio of R=14, indicates the alpha deformation texture as shown in Fig. 3. It is seen that alpha texture has 10-10 along the extrusion direction [17-18], which is distinct from the experiment texture in Fig. 1. The experimental texture shows that, however, 0001 along the extrusion direction, meaning deformation texture is not dominant in the final alpha texture.

Hence, in the following section, we take into account the beta-alpha transformation during the post-extrusion cooling process. First of all, we calculated the deformation texture of beta phase using the finite element model in Fig. 2, then calculate the alpha transformation texture according to the beta-alpha Burgers relationship. In this transformation process, we firstly assume no preference of alpha variant, i.e. 12 alpha variants have the same probability of occurrence, from which the alpha transformation can be obtained. Subsequently, the alpha transformation texture is summed up with the deformation texture by weight, to get the final alpha texture, as shown in Fig. 4. It is seen that predicted alpha texture has 0001 pole along the extrusion direction, which is consistent with Fig. 1. However, the texture intensity is only 3.5, lower than the experimental intensity of 7.3. Nevertheless, it shows that transformation alpha texture in the final alpha texture of extruded titanium.

The deviation of texture intensity in Fig. 4 against experimental indicates that alpha variant selection occurred during the beta-alpha transformation. It must be taken into account while computing the final extrusion texture. This is how we calculate the alpha extrusion texture. It is no doubt that beta-alpha transformation texture will greatly affect the final texture. The above simulation has indicated that alpha transformation texture is dominated by 0001 texture, while alpha deformation texture is
dominated by 10-10 texture. The weight of the abovementioned two components depends on forming temperature, or phase fraction. Different alpha variant selection rule will alter the final alpha extrusion texture 0001 intensity. Previous studies on the variant selection phenomena have reported a number of potential mechanisms, e.g. (i) the common {110} rule [14], i.e. the adjacent transformed β grains with common {110} pole will lead to preferential selection of α variants. Based on this variant selection rule, alpha transformation texture was calculated by numerically decomposing beta deformation texture according to α variant selection rule. The transformation texture was sum up with the deformation texture in Fig. 3 to obtain the final alpha texture shown in Fig. 5. It shows evident 0001 texture along the extrusion direction, with quite comparable intensity with the experimental result in Fig. 1. It also implies that the common {110} rule has high promise in describing the texture evolution associated with beta-alpha transformation [14].

5. Conclusions
By crystal plasticity finite element method, the hot extrusion texture of alpha-beta titanium alloy were studied. The following conclusions have been drawn:
1) The crystal plasticity modelling based toolbox is capable of predicting the deformation and transformation texture evolution of alpha and beta phase during extrusion.  
2) Alpha deformation texture has 10-10 along the extrusion direction, which is different from the 0001 alpha extrusion texture.  
3) Beta-alpha transformation during cooling must be considered, due to its effect on 0001 alpha transformation texture, which is dominant in the final alpha extrusion texture.  
4) Variant selection is important in the beta-alpha transformation process. By taking into account the transformation texture via proper alpha variant selection rule, the model can provide satisfactory prediction of extrusion texture. Future study will be centred on microscopic study of alpha variants experimentally in comparison with prediction.

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References
[1] Lütering G, Williams J C, Titanium, Berlin; New York: Springer, 2003, 15-22  
[2] Taylor G I. Plastic strain in metals. J Inst Metals, 1938, 62: 307-324
[3] Vanhoutte P. Simulation of rolling and shear texture of brass by taylor theory adapted for mechanical twinning. Acta Metall, 1978, 26(4): 591-604
[4] Honeff H, Mecking H, in: Nagashima S (Ed.) Proc. Int. Conf. on Texture Mater., 6th, The Iron and Steel Institute of Japan, 1981, 347-355
[5] Crumbach M, Pomana G, Wagner P, et al., in: G. G, D. M (Eds.) Recrystallization and Grain Growth Springer, Berlin, 2001, 1061-1068
[6] Lebensohn R A, Canova G R. A self-consistent approach for modelling texture development of two-phase polycrystals: Application to titanium alloys. Acta Mater, 1997, 45(9): 3687-3694
[7] Tomé C N, Lebensohn R A, Kocks U F. A model for texture development dominated by deformation twinning: Application to zirconium alloys. Acta Metall Mater, 1991, 39(11): 2667-2680
[8] Mayeur J R, McDowell D L. A three-dimensional crystal plasticity model for duplex Ti-6Al-4V. Int J Plasticity, 2007, 23(9): 1457-1485
[9] Kim D K, Kim J, Park W, et al. Three-dimensional crystal plasticity finite element analysis of microstructure and texture evolution during channel die compression of IF steel[J]. Comput Mater Sci, 2015, 100:52-60.
[10] Mayama T, Noda M, Chiba R, et al. Crystal plasticity analysis of texture development in magnesium alloy during extrusion. Int J Plasticity, 2011, 27(12): 1916-1935
[11] Yao J Y, Wang B S, Deng L P, et al. Simulation of texture evolution and deformation mechanism in Mg-3Al-1Zn alloy during uniaxial compression. Sci China: Tech Sci, 2015, 58(12): 2052-2059.
[12] Dunst D, Mecking H. Analysis of experimental and theoretical rolling textures of two-phase titanium alloys. Z Metallkd, 1996, 87(6): 498-507
[13] Glavicic M G, Goetz R L, Barker D R, et al. Modeling of texture evolution during hot forging of alpha/beta titanium alloys. Metall Mater Trans A, 2008, 39A(4): 887-896
[14] Bhattacharyya D, Viswanathan G B, Denkenberger R, et al. The role of crystallographic and geometrical relationships between alpha and beta phases in an alpha/beta titanium alloy. Acta Mater, 2003, 51(16): 4679-4691
[15] Hill R. On constitutive macro-variables for heterogeneous solids at finite strain [J]. Proceedings of the Royal Society of London, 1972, 326(1565): 131-147.
[16] Asaro R J. Micromechanics of Crystals and Polycrystals [J]. Advances in Appl Mech, 1983, 23(08): 1-115.
[17] Wei P T, Lu C, Tieu K, et al. Modelling of Texture Evolution in High Pressure Torsion by Crystal Plasticity Finite Element Method [J]. Applied Mechanics and Materials, 2015, 764-765:56-60.
[18] Sheik H, Ebrahimi R. Investigation on texture evolution during cyclic expansion-extrusion (CEE) technique using crystal plasticity finite element modeling [J]. J Mater Sci, 2016, 51(22): 10178-10190.