A novel method for predicting variant selection during primary, secondary and tertiary twinning in titanium

Lei Bao, Christophe Schuman, Qichi Le, Jean-Sébastien Lecomte, Zhiqiang Zhang, Marie-Jeanne Philippe, Jianzhong Cui, Claude Esling

A novel method for predicting variant selection during primary, secondary and tertiary twinning in titanium

Lei Bao [a,*] , Christophe Schuman [b], Qichi Le [a], Jean-Sébastien Lecomte [b], Zhiqiang Zhang [a], Marie-Jeanne Philippe [b], Jianzhong Cui [a], Claude Esling [b]

[a]Key Lab of Electromagnetic Processing of Materials, Ministry of Education, Northeastern University, Shenyang 110819, People′s Republic of China

[b]Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux, LEM3, CNRS UMR 7239, Université de Lorraine, Metz 57045, France

* Corresponding author. Tel.: +86 2483687734;fax: +86 2483681758.

E-mail address: baolei@epm.neu.edu.cn (L. Bao).

Highlights

●We propose a novel method based on Schmid′s law for predicting the twin variant selection in titanium.

●This method is proved to be a more effective criterion than Schmid′s law by comparing with the experimental results.

●This method effectively improves the accuracy to about 90% of predicting the primary, secondary and tertiary twinning variant selection.

Abstract

The present paper proposes a novel method based on Schmid′s law by introducing a calculation of "Normalized Schmid factor" as an indispensable criterion for predicting twin variant selection in commercially pure titanium. Through comparing the calculation with experimental results, this novel method is proved to be a more effective criterion than Schmid′s law and the accuracy is about 90% during primary, secondary and tertiary twinning variant selection.

Keywords : Titanium, Twin variant selection;, Schmid′s law, Crystal structure, Simulation and , modeling

1. Introduction

Mechanical twinning is a particularly important deformation mode in HCP metals that have limited number of slip systems [1], [2], [3], [4]. As the research on mechanical twinning of HCP metals continues, a number of experts concentrate themselves on the field of twin variant selection, and propose that several factors could have influence on twin variant selection during plastic deformation, such as Schmid factor (SF), potential for growth and total strain accommodation [5], [6], [7], [8], [9].

At present, it is well accepted that variant selection during primary twinning follows Schmid′s law. However, in the case of secondary twinning, Barnett, Jonas et al. and Mu et al. [7], [8], [9], [10] reported that Schmid′s law is not the only factor affecting variant selection, common volumes and primary to secondary accommodation shears would play more important roles.

For polycrystalline titanium, because of the difference in c/a ratio from that of magnesium, the twin variant selection during both of primary and secondary twinning is found to follow Schmid′s law well on the whole. Nevertheless, the accuracy of predicting twin variant selection by Schmid′s law is unacceptable due to some inevitable errors in the calculation of SF [11].

Consequently, to improve the accuracy of predicting the twin variant selection, the present paper proposes a novel method based on Schmid′s law. This method introduces “Normalized Schmid factor” (NSF) as an indispensable criterion for predicting the twin variant selection and we define this novel method as “SF–NSF method”. We compare the predictions by both of Schmid′s law and the SF–NSF method during the primary, secondary and tertiary twinning in commercially pure titanium with the result of a “Quasi-in-situ EBSD observation” experiment on uniaxial compression deformation.

2. Experimental

The material investigated is commercially pure titanium T40 sheet in the form of rolled sheet with the thickness of 1.5 mm. The detailed descriptions of “Quasi-in-situ EBSD observation” layout can be found in Ref. [11].

3. Results and discussions

As we know the traditional SF describes the resolved shear stress applied on twinning plane and to twinning direction under microscopic stress. For polycrystalline materials, the indices of twinning plane and twinning direction in macroscopic coordinate reference can be easily obtained through crystallographic calculations from the EBSD data of matrix grains [6]. However, the microscopic stress applied on the twin system is extremely difficult to be accurately acquired since neighboring grains, boundaries, texture, defects and precipitated particles can all affect the microscopic stress. Hence the common practice is using macroscopic stress instead of microscopic stress in the SF calculation. As a consequence of this replacement, the calculated SF is not accurate and would cause an incorrect SF ranking in the case that some of the potential twin variants have relatively close SFs. This is the primary problem of using Schmid′s law to predict the twin variant selection [11].

Therefore, to overcome the challenge, we propose a novel method based on Schmid′s law by proposing a calculation of NSF. As we know, a twin in HCP materials has six potential variants and the variant with the highest SF indicates that the highest resolved shear stress is applied on it among all the six variants. The aim of proposing the calculation of NSF is to give the quantitative information to the deviation of each variant′s resolved shear stress from the highest one. The NSF calculation is $NSF=SF_i/SF_h$, where SF_i represents the SF of the current variant and SF_h represents the highest SF among the six potential variants. If NSF equals to 1, it means that the current variant is the highest SF variant; if NSF is less than 1, the NSF then provides information about to what extent the SF of the current variant deviates from the highest SF.

We analyze the SF and the NSF for each potential primary, secondary and tertiary twin variant in 100 twinned grains and compare them with the experimental result. The frequency of the active primary twin variants ranked by the SF corresponding to the six potential primary twin variants is calculated and shown in Fig. 1, where "1" is the highest and "6" is the lowest in the SF. It is seen that the 43% active twin variants have the 1st ranking SF, and 30% active twin variants have the 2nd ranking SF from Fig. 1a. Therefore, the accuracy of predicting twin variant using Schmid′s law is only 43% that is not acceptable. In Fig. 1b, clearly we can see that 91% active variants have the NSF higher than 0.83, which demonstrates that the majority of twin variants with the non-highest SF can be activated on condition that their SFs are relatively close to the highest SF. Consequently it is reasonable to assume that the replacement of microscopic stress by macroscopic stress probably reverses the SF ranks of some of variants whose NSFs are higher than 0.83.

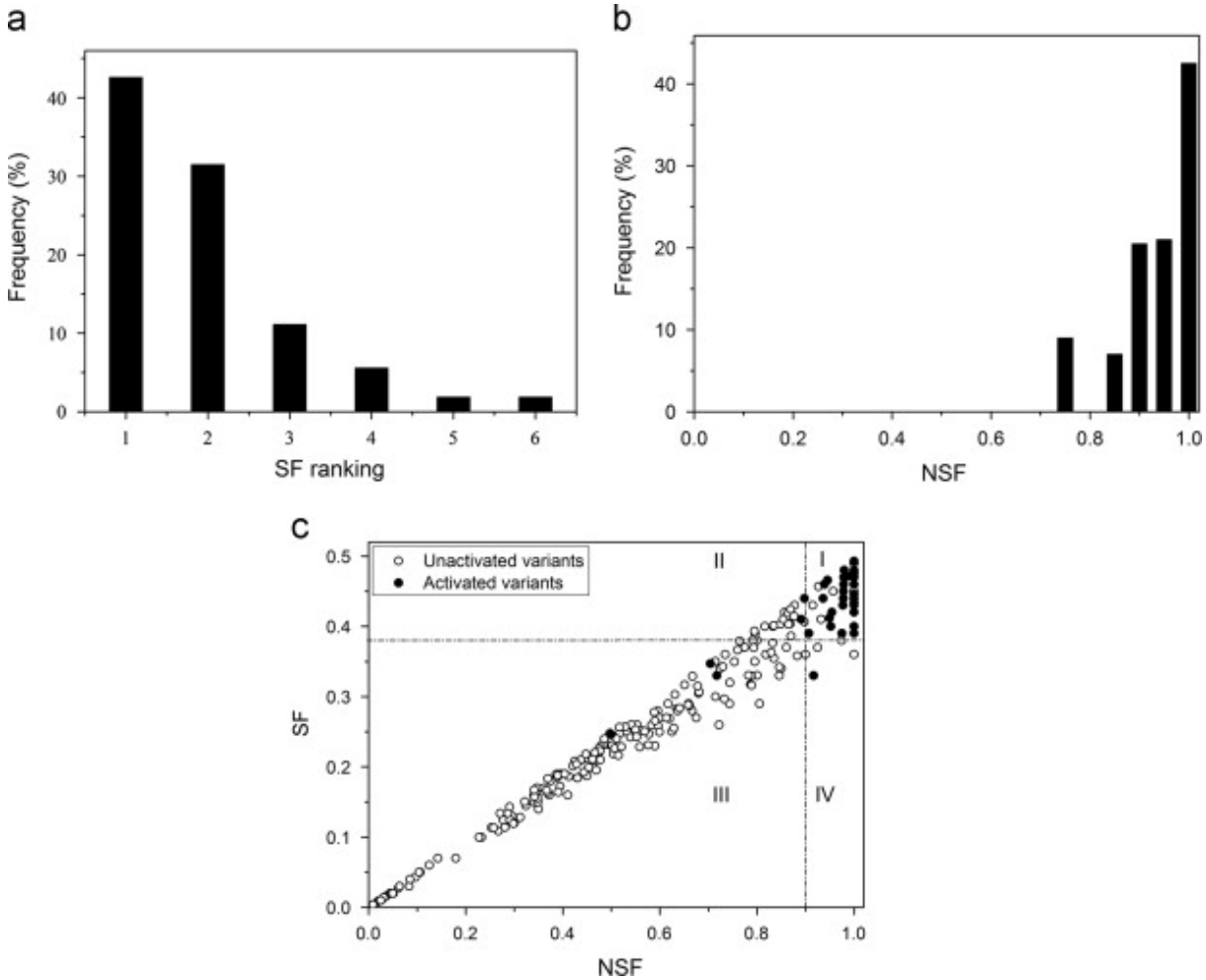

Fig. 1. *(a) Frequency of the active primary twin variants in function of their SF rank with respect to the SF of the 6 potential variants (here "1" is the highest and "6" is the lowest), (b) Frequency of the active primary twin variants in function of their NSF and (c) Scatter diagram of primary potential twin variants on the NSF–SF coordinate (inactivated variants represented by vacant spots and activated variants represented by solid spots).*

The operation of the SF–NSF method is firstly to build a rectangular coordinate with NSF as the horizontal axis and SF as the vertical axis, and then divide this NSF–SF coordinate into four quadrants by two reference lines of SF equals to 0.38 and NSF equals to 0.90. Next, scatter all calculated variants on this NSF–SF coordinate as shown in Fig. 1c, where vacant spots represent inactivated variants and solid spots represent activated variants. One of the

interesting findings in Fig. 1c is that 90% variants within quadrant I are activated, and it is reasonable to deduce that the SF greater than 0.38 and the NSF greater than 0.90 (the quadrants I in Fig. 1c) is a better criterion of predicting the variant selection with a satisfactory accuracy of 90%.

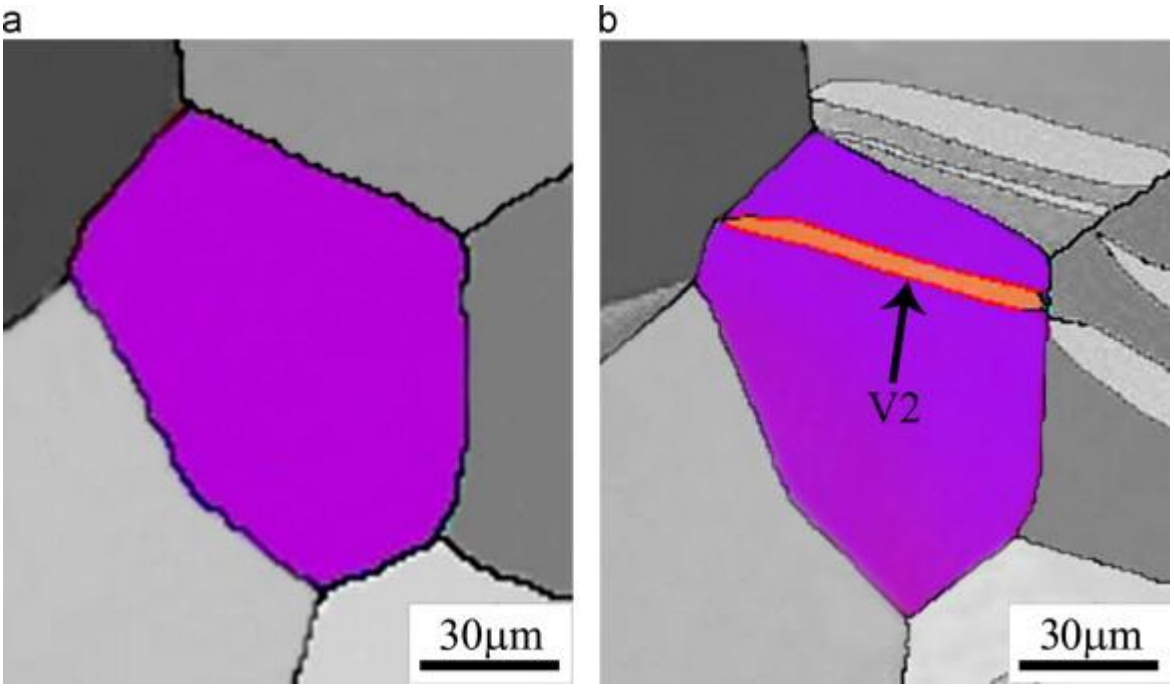

Fig. 2. *A grain in the (a) initial state and (b) 8% compressive deformation.*

Fig. 2 shows two OIM images by "Quasi-in-situ EBSD observation". The initial state of the matrix grain is given in Fig. 2a. The SFs and the NSFs of the six potential {} twin variants are calculated according to the crystallographic orientation of the matrix grain and the macroscopic stress (see Table 1). Note that in the matrix grain after 8% compressive deformation shown in Fig. 2b, the activated variant is not the one with the highest SF (V1 in Table 1), but the one with the 2nd ranking SF of 0.45 and a very high NSF of 0.96 (V2 in Table 1). In this case, the SF–NSF method identifies V2 as a high-probability variant, inversely, Schmid′s law identifies it as a low-probability variant since it is not the highest SF variant.

The SF rank and the NSF for the secondary and the tertiary twinning were also examined and are shown together in Fig. 3, where the secondary variants are presented in blue and the tertiary variants are presented in red. From the information given in Fig. 3, 88% variants in quadrant I are activated, which is not significantly different from the accuracy of the primary twinning. Fig. 4 shows a grain with secondary and tertiary twinning. The 2nd and the 3rd columns of Table 1 list the SFs and the NSFs for all the potential secondary and tertiary variants of the grain in Fig. 4. The activated secondary and tertiary variants both have very high NSF but not the highest SF, which is quite similar to the situation of the primary twinning shown in Fig. 1. Thus we can conclude that the NSF–SF method is still valid for secondary and the tertiary twinning.

Table 1. *SFs and NSFs of the six potential twin variants of the grains shown in Fig. 2, Fig. 4.*

Potential variants	SF	NSF	Potential variants	SF	NSF	Potential variants	SF	NSF
V1: Variant $(11\bar{2}2)$	0.47	1.00	V1: Variant $(10\bar{1}2)$	0.01	0.02	V1: Variant $(11\bar{2}2)$	0.23	0.47
V2: Variant $(\bar{1}2\bar{1}2)$	0.45	0.96	V2: Variant $(01\bar{1}2)$	0.43	1.00	V2: Variant $(\bar{1}2\bar{1}2)$	0.21	0.43
V3: Variant $(\bar{2}\bar{1}12)$	0.34	0.72	V3: Variant $(\bar{1}102)$	0.29	0.67	V3: Variant $(\bar{2}112)$	0.38	0.79
V4: Variant $(\bar{2}\bar{1}12)$	0.19	0.40	V4: Variant $(\bar{1}012)$	0.01	0.02	V4: Variant $(\bar{2}\bar{1}12)$	0.47	0.98
V5: Variant $(1\bar{2}12)$	0.26	0.55	V5: Variant $(0\bar{1}12)$	0.42	0.98	V5: Variant $(1\bar{2}12)$	0.48	1.00
V6: Variant $(2\bar{1}\bar{1}2)$	0.33	0.70	V6: Variant $(1\bar{1}02)$	0.27	0.63	V6: Variant $(2\bar{1}\bar{1}2)$	0.40	0.83

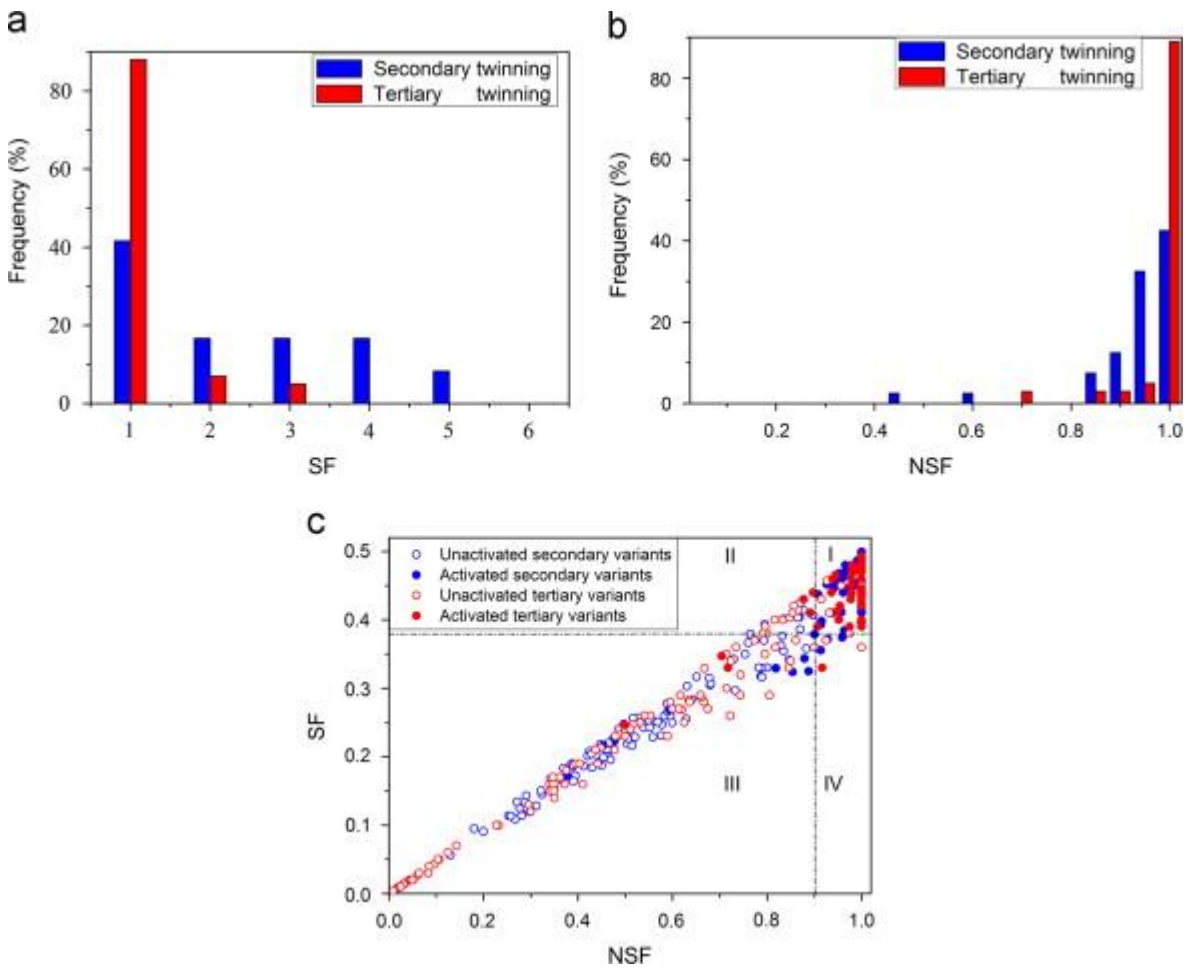

Fig. 3. *(a) Frequency of the active secondary and tertiary twin variants in function of their SF rank with respect to the SF of the 6 potential variants (here "1" is the highest and "6" is the lowest), (b) Frequency of the active secondary and tertiary twin variants in function of their NSF and (c) Scatter diagram of active secondary and tertiary twin variants on the NSF–SF coordinate.*

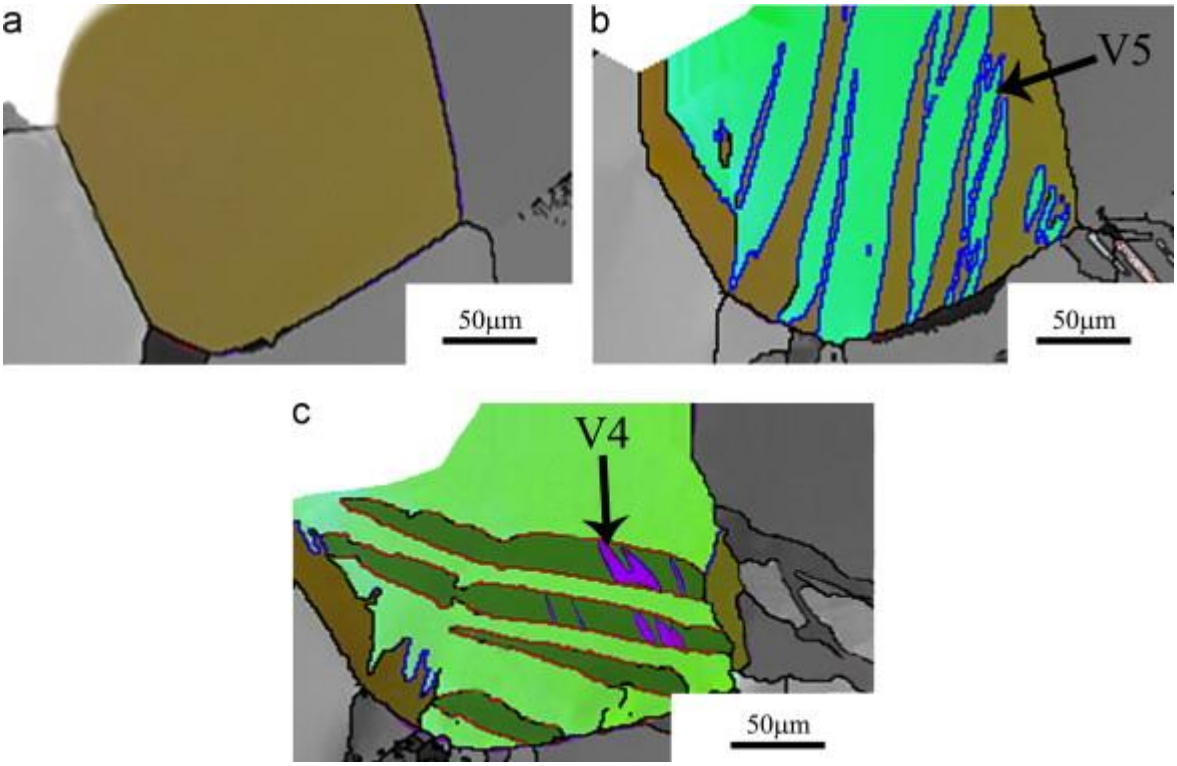

Fig. 4. *A grain in the (a) initial state, (b) 8% and (c) 16% compressive deformation.*

Figs. 1(c) and 3(c) reveal two kinds of errors reducing the accuracy of this method. The first error is that several unexpected low NSF twin variants were activated in non-quadrant I, and the second error is that several predicted variants were not activated. In another word, the first error causes some variants "observed but not predicted", and the second error causes some variants "predicted but not observed".

During plastic deformation, stress concentration is inevitable because of the inhomogeneity of plastic deformation in polycrystalline metals. The microscopic stress thus probably deviates greatly from the macroscopic stress under the effect of severe stress concentration, so the calculated SF and NSF are far from the true values and cause the first error of this SF–NSF method. The first error reduces the accuracy by less than 5% according to the statistical result, but unfortunately this percentage will increase during higher plastic deformation because of the severe stress concentration.

The second error is mainly caused by the competitive mechanism among twin variants. Generally, in one grain, there may exist several predicted variants in quadrant I. Once the most competitive variant has been activated, then the local energy is released, and the other predicted variants in this grain do not have the required local energy to be activated. This error reduces the accuracy by approximately 5–10%, and it can be avoided by adding an additional criterion to exclude the other predicted variants belonging to one same grain within quadrant I.

In brief, the limitation of this method is that the high plastic deformation causes the first error and the competitive mechanism causes the second error. Consequently, we recommend readers adopting this method under relatively low plastic deformation and using an additional criterion to reduce the second error.

4. Conclusions

In summary, according to the comparison with the experimental results, the NSF–SF method is proved to be a more effective criterion than Schmid′s law. It could allow us to avoid the error in the calculation of the SF to a large extent, and effectively improve the accuracy to about 90% of predicting the primary, secondary and tertiary twinning variant selection.

Acknowledgments

The authors are grateful to the financial support from the Major State Basic Research Development Program of China (2013CB632203), the Fundamental Research Funds for the Central Universities (N120309003 and N120509002), the Program for Liaoning Excellent Talents in University (LJQ2012023), the Liaoning Provincial Natural Science Foundation of China (201202072) and the Federation of Research for Aeronautic and Space – Fédération de Recherche pour l′Aéronautique et l′Espace Thème Matériaux pour l′Aéronautique et l′Espace: project OPTIMIST (optimization de la mise en forme d′alliage de titane).

References

[1] P Vedoya, A Pochettino, R Penelle, Texture Microstruct, 8 (1988), pp. 601-610
[2] MJ Philippe, M Serghat, P Van Houtte, C Esling, Acta Metall, 43 (1995), pp. 1619-1630
[3] JJ Fundenberger, MJ Philippe, F Wagner, C Esling, Acta Mater, 45 (1997), pp. 4041-4155
[4] S Zaefferer, Mater Sci Eng A, 344 (2003), pp. 20-30
[5] H Miura, T Sakai, J.J Jonas, Scr Mater, 55 (2006), pp. 167-170
[6] S Godet, L Jiang, AA Luo, JJ Jonas, Scr Mater, 55 (2006), pp. 1055-1058
[7] E Martin, L Capolungo, L Jiang, J.J Jonas, Acta Mater, 58 (2010), pp. 3970-3983
[8] JJ Jonas, S Mu, T Al-Samman, G Gottstein, L Jiang, E Martin, Acta Mater, 59 (2011), pp. 2046-2056
[9] S Mu, JJ Jonas, G Gottstein, Acta Mater, 60 (2012), pp. 2043-2053
[10] MR Barnett, Z Keshavarz, AG Beer, X Ma, Acta Mater (2008), pp. 5-15
[11] L Bao, Y Zhang, C Schuman, JS Lecomte, MJ Philippe, X Zhao, *et al.*, J Appl Cryst, 46 (2013), pp. 1397-1406