DYNAMIC HARDENING RULE; A GENERALIZATION OF THE CLASSICAL HARDENING RULE FOR CRYSTAL PLASTICITY

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Abstract

The mechanical properties of a niobium (Nb) tensile specimen can vary with the orientation of the tensile axis. This anisotropy causes inhomogeneity in manufactured SRF cavities. Large grain Nb slices from an ingot are more anisotropic and less expensive than fine grain sheets. Designing an optimal manufacturing process for large grain Nb sheets, however, is complex, and requires use of advanced modeling techniques.

A model capable of accurately predicting the deformation behavior of Nb can be used to improve the performance and reduce costs of a SRF cavity. Ultimately, optimal design of a manufacturing process with tube hydroforming is possible with such a model.

Crystal plasticity modeling of FCC materials has been very successful; however, there is still no model that can accurately predict the deformation behavior of single crystal BCC materials like the large grain Nb slices.

In this study, a dynamic hardening rule for crystal plasticity is presented that significantly improves predictions of the stress-strain deformation of single crystal Nb. This model is a generalization of the classical hardening rule, and gives better control over the hardening rate. It also increases the stability of the model.

INTRODUCTION

Nb is widely used in manufacturing polycrystalline SRF cavities, but the origins of the variability in its mechanical properties are not well-understood. Nb is very anisotropic and its mechanical response depends greatly on the direction of loading with respect to its crystal orientation. This anisotropy complicates the design of a manufacturing process. One way to deal with this problem is to use sheet Nb with randomly oriented fine grains, but these are not easily achieved. Cavities made from large grain slices from ingots, however, can provide similar or better SRF performance [1]. They are also less expensive due to not going through the rolling process.

Although the combination of cost and performance makes large grain sheets a desirable candidate, the difficulties caused by their anisotropic deformation has restricted their application. A model capable of predicting the deformation behavior of Nb can help facilitate designing a manufacturing process for large grain cavities. Such a model can be implemented in Computer Aided Design/Evaluation (CAD/CAE) software and be used to design a manufacturing process.

Modeling deformation behavior of materials has long attracted researchers[2–7]; nevertheless, modeling of deformation of Nb has not received much attention.

Crystal plasticity is one of the modeling strategies that can be used to predict the deformation behavior of metals. Although conventional crystal plasticity models work relatively well for FCC materials and BCC polycrystals, their performance is not accurate enough for different orientations of single crystal BCC.

In this study a generalized dynamic hardening model is developed that, when implemented in a crystal plasticity scheme, can improve the accuracy of results.

DEVELOPING THE CRYSTAL PLASTICTY MODEL

Crystal plasticity theory assumes that deformation is a result of application of stresses higher than a critical value and happens only due to dislocation slip on slip planes. The crystal plasticity model used in this study is developed from the work of Zamiri and Pourborghrat [6]. In this model they additively decompose the deformation gradient to elastic and plastic parts, and define a yield function to estimate the onset of yielding. For their hardening model they follow Asaro's [8] approach:

$$\dot{\tau}^{\alpha}_{Class} = \sum_{\beta=1}^{N} h^{\alpha\beta}\left|\dot{\gamma}^{\beta}\right| \qquad (1)$$

in which $\dot{\tau}^{\alpha}_{\mathrm{Class}}$ is the increment in shear stress for a slip system α, $\dot{\gamma}^{\beta}$ is the increment of shear strain on a slip system β and $h^{\alpha\beta}$ is defined as follows:

$$h^{\alpha\beta} = h^{\beta}\left[q + (1-q)\delta^{\alpha\beta}\right] \qquad (2)$$

Where $\delta^{\alpha\beta}$ is the Kronecker's delta, $1 \leq q \leq 1.4$, and h^{β} is defined as:

$$h^{\beta} = h_0\left|1 - \frac{\tau_y^{\beta}}{\tau_s}\right|^{a} sgn\left(1 - \frac{\tau_y^{\beta}}{\tau_s}\right), \qquad (3)$$

in which h_0 is the initial hardening rate, a is the hardening exponent and τ_s is the saturation value of hardening and τ_y^{β} is the current critical resolved shear stress on a slip system β.

The crystal plasticity model with the above hardening model was calibrated for a crystal orientation P shown in Figure 1(a), and then was used to predict the deformation behavior of another crystal orientation named S. Figure 2 shows the results of tensile tests and simulations for these two as-cast crystal orientations. Since the model was calibrated for P orientation, the simulated P stress-strain curve closely matches with the experiment. But the prediction of stress for S is even higher than that of the P orientation, while in reality S is a softer orientation.

Although this model accurately predicts the deformation of FCC single and polycrystals [6], its results are not satisfactory for BCC single crystals.

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To address this problem, a generalized dynamic hardening model was developed which improved the prediction of the crystal plasticity model. In a special case, this hardening model reduces to equation (1). This paper compares the results of the classical hardening rule and the dynamic hardening rule for annealed Nb samples.

Dynamic Hardening Rule

In BCC materials, deformation takes place as a result of dislocation slip on 48 independent slip systems. During the deformation these slip systems interact with each other and harden the material. The classical hardening rule, equation (1), assumes that all concurrently active slip systems harden simultaneously with different rates. This assumption may be true for some conditions, but it fails to consider the effect of slip history on a slip system, or the lack of neighboring grain constraint that is present in a single crystal.

Let us assume that at the beginning of deformation of a single crystal, only one slip system is activated. This slip system, therefore, only hardens as a result of interaction with the pre-existing dislocation forest dislocations, which may be few if the material is well annealed. Dislocations close to a surface can easily exit the material without overcoming many obstacles. As the deformation proceeds, the crystal rotates, making other slip systems more favorable, and are eventually activated. Increasing the number active slip systems, in turn, increases the rate of hardening due to the presence of interactions with forest dislocations with different slip vectors. To capture this idea, equation (1) is multiplied by the following term:

$$\left((1-w)+w\left(\frac{\gamma^{2nd}}{\gamma^{1st}}\right)^{n}\right) \qquad (4)$$

In the above equation w and n are a weight factor and dynamic hardening exponent, respectively. γ^{1st}, γ^{2nd} are the accumulated shear stress on the most active and the second most active slip system. The term $w\left(\frac{\gamma^{2nd}}{\gamma^{1st}}\right)^{n}$ evaluates the effect of total slip activity on the first and second most active slip systems. When one slip system is considerably more active than the others this ratio is close to zero; and consequently, this slip activity does not contribute much to hardening. The more other slip systems activate, the more this ratio grows, and the more it adds to the hardening rate in the model. The term $(1-w)$ is in place to model the hardening that comes from the dislocation forest, which exists at the beginning of the deformation. A weight factor w, is introduced to adjust the relative contribution of each term. The exponent n is a material parameter that can control the effect of the slip ratio. The final form of the so called Dynamic hardening rule is as below:

$$\dot{\tau}^{\alpha}_{\mathrm{Dyn}}=\sum_{\beta=1}^{N} h^{\alpha\beta}\left|\dot{\gamma}^{\beta}\right|\left((1-w)+w\left(\frac{\gamma^{2nd}}{\gamma^{1st}}\right)^{n}\right) \qquad (5)$$

This is the generalized form of the hardening law presented in [7]. For $n=0$ this model reduces the classical hardening model, equation (1).

CALIBRATING THE MODEL

Tensile tests were used to calibrate the crystal plasticity models. Triplicate tensile samples with four different crystal orientations were cut from a Nb slice. The disk itself was cut from a high purity Nb ingot [9,10]. Samples that were cut directly from the ingot as well as samples with the same orientation, but annealed at 800°C, 2hr were deformed, and compared, as described in greater detail in [11]. The samples named “Q”, “R”, “T” and “W” were cut to favor different slip systems at the yield stress. Figure 1(a) shows the tensile axis of the samples. The finite element mesh used in simulations has the same geometry as the tensile samples. Figure 1(b) shows the deformed mesh for the W orientation, as simulated with the dynamic hardening model.

These tensile samples illustrated in Figure 2 have a high pre-existing dislocation density, which is introduced by the solidification process. Pre-existing dislocations increase the yield point and hardening rate of the material. Since the crystal plasticity model studied here does not directly consider the effect of pre-exiting dislocations (although their effect can be modeled through other parameters implemented in the code, like initial critical resolved shear stress.), the tensile samples presented in Figures 3-9 were annealed before the test. Figure 3 compares the stress-strain response of the R crystal orientation before and after annealing. Annealing considerably lowers the stress-strain curve, indicating that a high pre-existing dislocation density was removed, and softened the material. The model was calibrated for the W crystal orientation and then used to predict the stress-strain curve for other orientations.

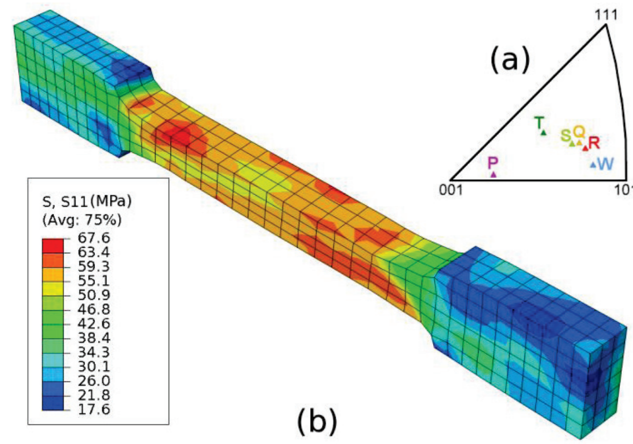

Figure 1(a): The tensile axis of samples used in this study. (b): Simulated deformation of W orientation with the Dynamic hardening model.

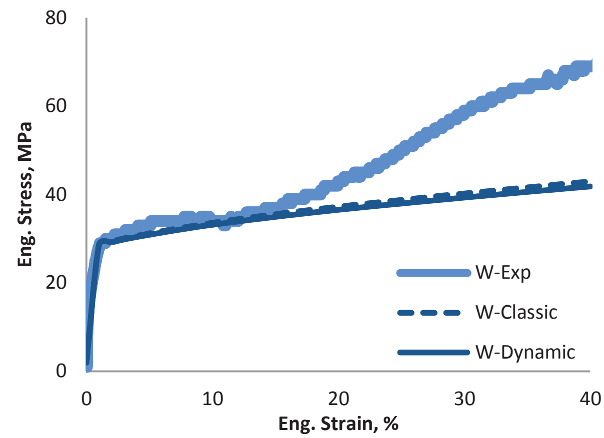

Figure 4: W orientation is used to calibrate both classical and Dynamic hardening models.

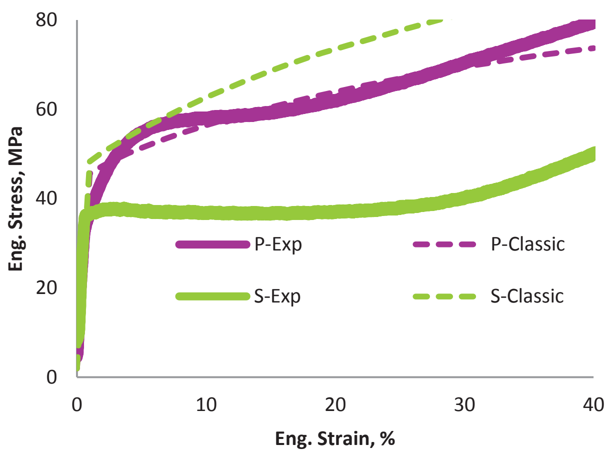

Figure 2: A classical hardening rule cannot predict the deformation behavior of two different crystal orientations of Nb cut directly from an ingot. The model was calibrated for the P orientation and then used for predicting the deformation of S orientation.

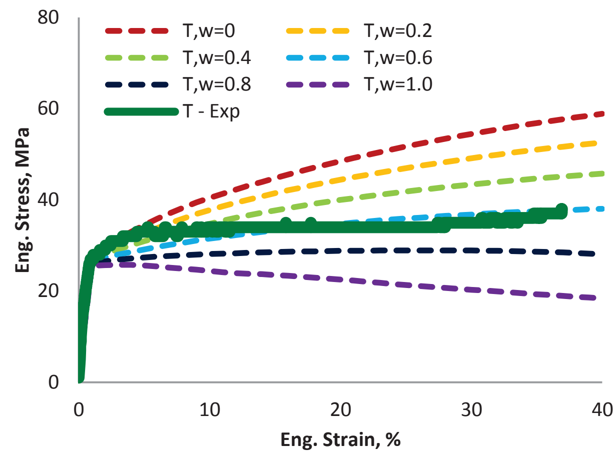

Figure 5: Predictions of the Dynamic Hardening rule with weight factors w between 0 and 1. $w = 0$ overestimates and $w = 1$ underestimates the hardening The solid line shows the experimental results for T orientation.

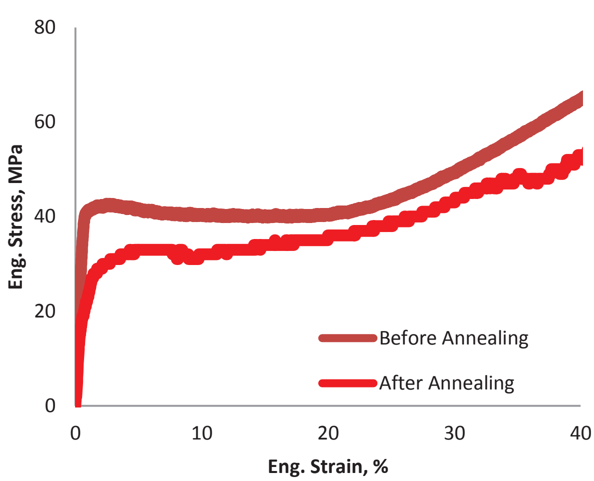

Figure 3: The effect of annealing on the engineering stress-strain response of an Nb tensile sample (Material Orientation R).

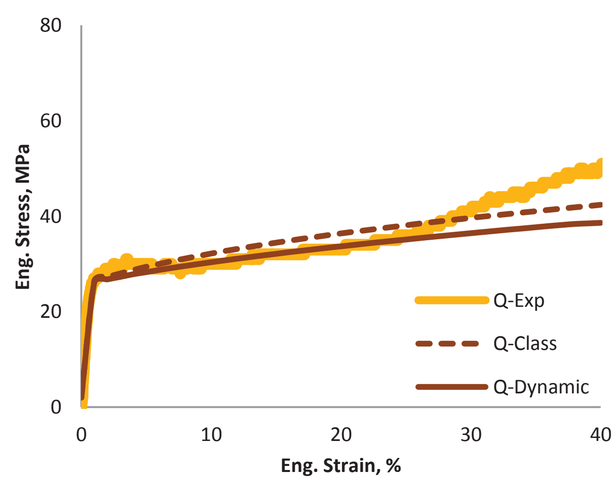

Figure 6: Prediction of both models for Q orientation.

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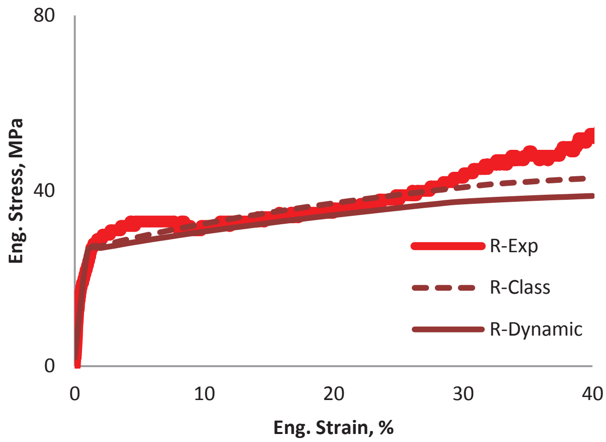

Figure 7: Prediction of both models for R orientation.

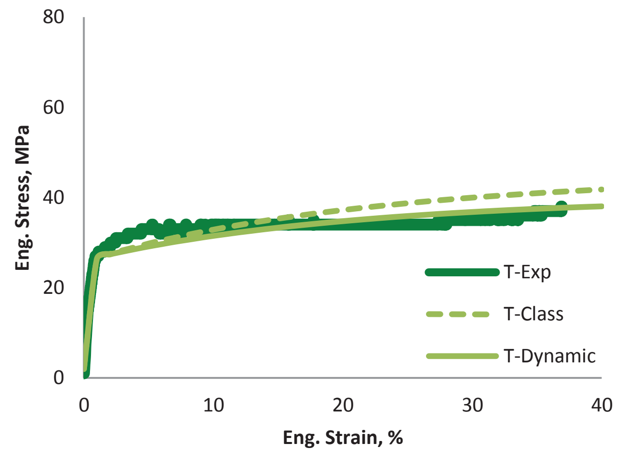

Figure 8: Prediction of both models for T orientation.

DISCUSSION

Both the classical hardening model and the dynamic hardening model were calibrated using the W orientation, and this is shown in Figure 4. The light blue line shows the experimental results, the solid navy blue line shows the predictions of the dynamic hardening model and the dashed navy blue line shows the simulation results for classical hardening model. The calibration of both models allow a good agreement with the experimental data up to a strain of about 20%. The weight factor $w = 0.6$ was used to calibrate the dynamic hardening model.

The classical hardening rule, equation (1) which corresponds to $w = 0$ in the dynamic hardening model, over estimates the stress-strain behavior for Nb, as discussed in [7]. The predictions of the dynamic hardening model with $w = 1$, on the other hand, leads to flow behavior that is softer than the experiments. In fact the experimental results usually fall between these two extremes. Figure 5 illustrates the effect of different values of w on the predictions of the dynamic hardening rule for the tensile sample T.

Figures 6, 7 and 8 show the predictions for both models for different crystal orientations. The models do not capture the increase in hardening rate that occurs later in the flow curve, a feature than needs further examination. The predictions of the dynamic hardening model are slightly better than those of the classical hardening mode.

The classical hardening model only considers the effect of resolved shear stresses and the increment of shear strain in modeling the hardening (see equations (1), (2) and (3)). The dynamic hardening model; however, considers not only these parameters but also the accumulated activity of the most active slip systems. Therefore, the dynamic hardening model reduces the hardening rate at the beginning of the deformation. As the deformation continues, the activity of slip systems increase and the hardening rate increases.

Figure 9 shows the results of all tensile tests and figure 10 shows the model simulations of the same tests on a plot with the same scales. The order of harder and softer orientations match, but the spread in the model is much smaller than the experiment, and the change in slope in the experiment at later strains is not captured. Further research is needed to determine how well the crystal rotations in the model compare to the experiments, to ascertain how well the model captures rotations.

CONCLUSION

The dynamic hardening rule considers the lace of accumulated dislocation storage for the most active slip systems in the hardening model, in addition to other parameters implemented in the classical hardening rule. This improves the accuracy of the model in prediction of deformation, and gives more control over the calibration process. Some parameters like the exponent n and weight factor w in the Dynamic hardening model can be used to fine tune the predictions of the model.

The difference between the accuracy of the classical hardening rule and the dynamic hardening model for annealed samples is small. But it seems that the Dynamic hardening rule is more accurate when used for modeling the as-cast samples.

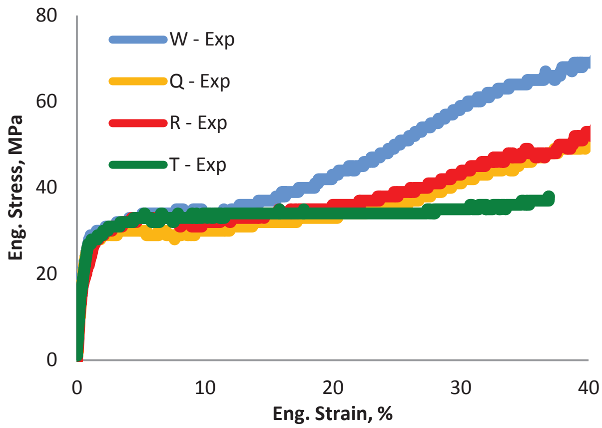

Figure 9: Comparison of tensile experiments of four annealed samples.

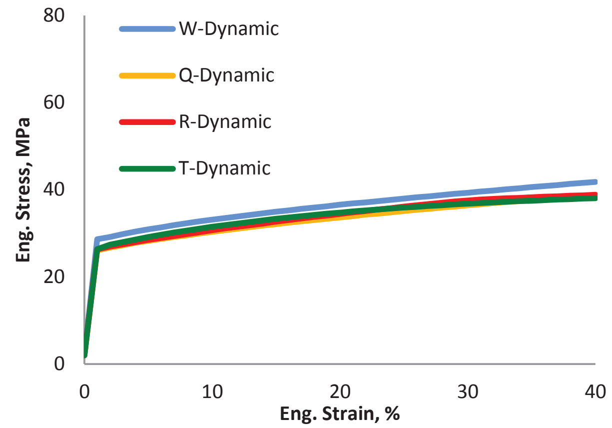

Figure 10: Comparison of modeling of four tensile tests with the dynamic hardening rule.

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REFERENCES

[1] Lee PJ, Polyanskii a. a., Gurevich a., Squitieri a. a., Larbalestier DC, Bauer PC, Boffo C, Edwards HT. Physica C: Superconductivity 2006;441:126.
[2] Hollomon JH. Metals Technoloogy 1945:268.
[3] Hill R. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1948;193:281.
[4] Barlat F, Lian J. Internationa 1989;5:51.
[5] Taylor GI. Twenty-Eighth May Lecture to the Institute of Metals 1938.
[6] Zamiri AR, Pourboghrat F. International Journal of Plasticity 2010;26:731.
[7] Mapar A, Bieler TR, Pourboghrat F, Compton CC. Crystal Plasticity Finite Element Modeling of Single Crystal Niobium Tensile Tests with Weighted Dynamic Hardening Rule, in: Li M, Campbell C, Thornton K, Holm E, Gumbsch P (Eds.). 2nd World Congress on Integrated Computational Materials Engineering. TMS (The Minerals, Metals & Materials Society); 2013.
[8] Asaro RJ. Journal of Applied Mechanics 1983;50:921.
[9] Baars D. Investigation Of Active Slip Systems In High Purity Single Crystal Niobium. Michigan State University, 2013.
[10] Bieler TR, Wright NT, Pourboghrat F, Compton C, Hartwig KT, Baars D, Zamiri a., Chandrasekaran S, Darbandi P, Jiang H, Skoug E, Balachandran S, Ice GE, Liu W. Physical Review Special Topics - Accelerators and Beams 2010;13:031002.
[11] Kang D, Baars DC, Bieler TR, Compton CC. Study of Slip in High Purity Single Crystal NB for Accelerator Cavities, TUP017, This proceeding, France: 2013.