

# Simulation of Duplex Heat Treatment Nb<sub>3</sub>Sn Compounds in Cu-Nb-Sn Superconducting Multifilamentary Wire

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## Abstract :

Nb<sub>3</sub>Sn is intermetallic compounds being used as superconductor formed by diffusion of Sn through grain boundary during internal tin process. It was known that grain boundary diffusion is dominant among any other mechanism. Numerical approached by finite difference method is used to study the distribution concentration of Sn. The present study focused on duplex heat treatment process i.e. it consists of two step heat treatments. Temperature and time of heat treatments were varied between 675-800oC and 32-200 hours, respectively. Duplex heat treatment can increase the Nb<sub>3</sub>Sn layer thickness, with the optimum increase was obtained as the first heat treatment temperature was set to be lower than that of the second one. The growth of the Nb<sub>3</sub>Sn at the Nb<sub>3</sub>Sn-Nb boundary depends largely on the concentration Sn at the grain boundaries.

**Keywords:** duplex heat treatment, finite difference method, grain boundary diffusion, intermetallic compound.

## 1. Introduction

Nb<sub>3</sub>Sn is intermetallic compound being used as multifilamentary superconducting composite conductors with A15 structure [1]. Nb<sub>3</sub>Sn is a brittle and has a composition range near stoichiometry over which properties vary, posing numerous production challenges. Even after over half a century of investigation, Nb<sub>3</sub>Sn still demands detailed study to optimize the conductors. Optimization of the heat treatment is, however, challenging since a lot of aspects may influence the properties of the conductors, such as the initial Nb and Sn contents, the geometry of the wire, additional elements and so on [2].

Reddi proposed a model for the A15 layer growth, where the growth rate is propotional to the Sn content in bronze [3]. At higher temperatures grain growth is predominant, and the growth rate is faster. At lower temperatures the nucleation of new grains takes over, and the growth rate is slower. Despite the fact of grain growth, grain boundaries (GB's) are known to provide easy paths for mass transport in materials since the energies of defect formation and migration in GB's tend to be lower than in the bulk lattice [4]. GB diffusion is a technologically important topic. Kinetics of many microstructural changes, phase transformations, and solid state reactions in engineering materials are often controlled by GB diffusion. In the field of solid state reaction, the GB diffusion allows the rate of growth deviates from the parabolic time dependence [5]. Earlier findings have studied the growth of Nb<sub>3</sub>Sn intermetallic layers through grain boundary diffusion [6].

Understanding the most important factors involved in the formation and growth of Nb<sub>3</sub>Sn will contribute to the improvement of its superconducting properties allowing better choices for the heat treatment parameters. This research focused on heat treatment optimization in internal tin manufacturing process, particularly on duplex (two step) heat treatment of internal tin process. The influence of the low and/or high temperature heat treatment steps on diffusion and phase formation is discussed.

## 2. Material and Methods

The model used by Fisher [7] to describe diffusion along the GBs comprises the free surface carrying the diffusion source (C<sub>0</sub>) and the GB being perpendicular to that surface. The GB has a constant thickness 2a (Fig.1), i.e. represents a slab, with the diffusion coefficient D' remaining constant along the GB. Fisher's model, known also as the isolated boundary model, represents a typical 2D semi-infinite problem. The concentrations and fluxes

coincide at the boundaries separating the GB and the grain, i.e. at  $x=a$ , allowing the leakage of atoms that exists from the GB into the grain to be taken into account. Consequently, Fisher's model is based on the assumption that  $D' \gg D$  ( $D$  is diffusion coefficient in the grain). Fisher model was then solved analytically by Whipple [8] and the formalism was then applied by Farrell et al [6]:

And the boundary condition :

$$D \nabla^2 C = \frac{\partial C}{\partial t} \quad [1]$$

$$D' \frac{\partial^2 C}{\partial y^2} + \frac{D}{\alpha} \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}, x = 0 \quad [2]$$

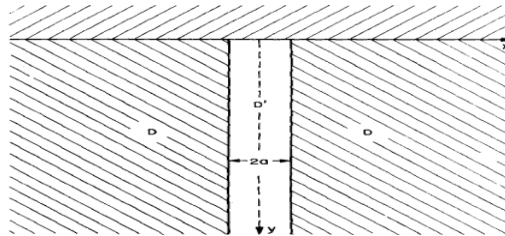


Figure 1. Model of isolated grain with grain boundary width of  $2a$  [6].

During duplex (two-step) heat treatment it is assumed that the diffusion flux will occur as shown in Fig. 2. Sn is assumed being located at GBs and the diffusion of Sn is the only mechanism. The diffusion fluxes are only driven by the flux of Sn towards  $Nb_3Sn$  that was formed during the first step heat treatment and diffusion of Sn in  $Nb_3Sn$  to Nb grain. As reservoir Sn at the GBs has concentration of  $C_0$  (initial concentration of Sn), for the present condition it is set as 0.2 [9]. For Sn in  $Nb_3Sn$  being diffused to Nb grain, the  $C_0$  is equal to  $C_1$  (concentration of Sn in  $Nb_3Sn$ ). Thus, total layer thickness of  $Nb_3Sn$  produced may consist of two sub-layers, i.e.  $Y_{o Sn-Nb_3Sn}$  and  $Y_{o Nb_3Sn-Nb}$

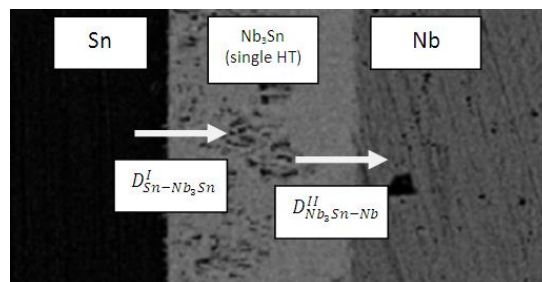


Figure 2. Model of diffusion process in duplex heat treatment

The  $Nb_3Sn$  sub-layers are calculated sequentially by using implicit finite difference method. The equation is derived from equation (2) as follows:

$$\frac{1}{\Delta t} C_j^n = -C_{j-1}^{n+1} \left( \frac{D}{\Delta y^2} \right) + C_j^{n+1} \left( \frac{2D}{\Delta y^2} + \frac{1}{\Delta t} \right) - C_{j+1}^{n+1} \left( \frac{D}{\Delta y^2} \right) \quad [3]$$

Diffusion coefficient of Sn in Nb is estimated through [10] with  $g$  being dimensionless parameter

$$k = g \sqrt{4Dt} \quad [4]$$

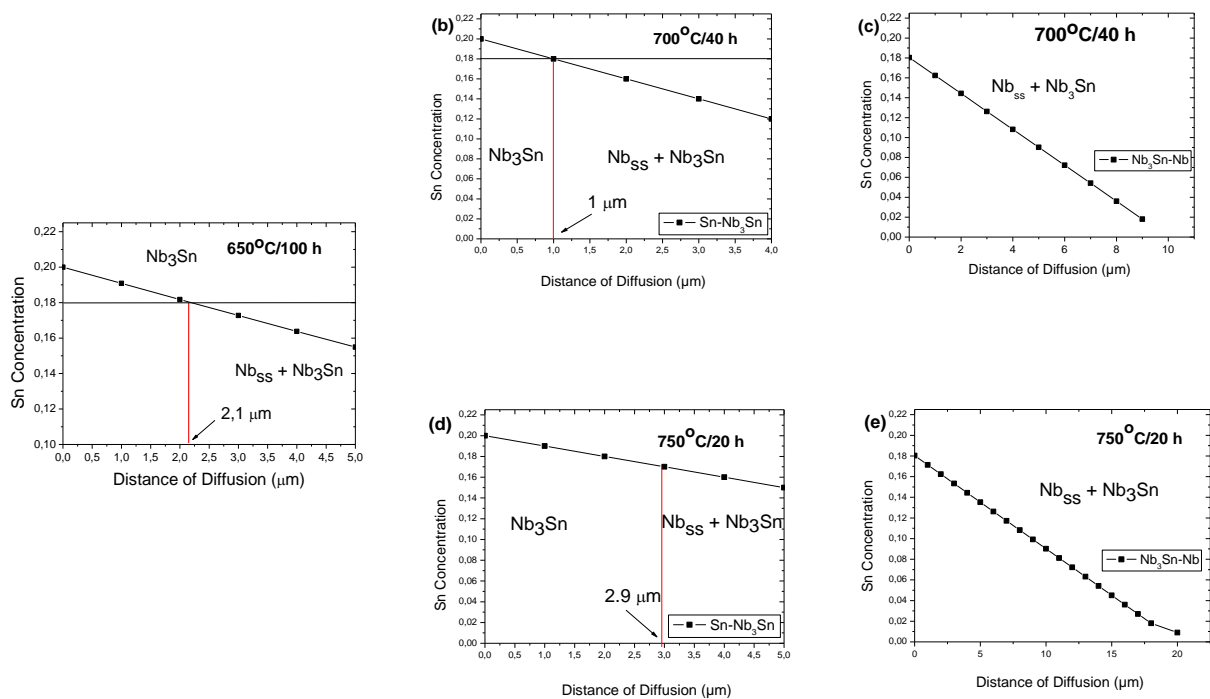
Diffusion coefficient of Sn in  $Nb_3Sn$  uses [6]

$$D = 0,022 \exp \left[ -\frac{55000}{RT} \right] \quad [5]$$

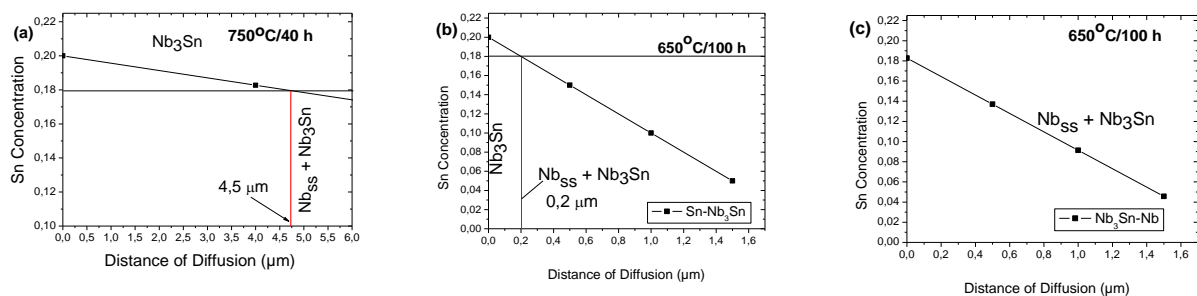
With:  $R$  is gas constant (1,97 cal/(mol.K), and  $T$  is temperature of diffusion (K)

### 3. Result and Discussion.

Figure 3 shows the simulation results for heat treatments at 650°C for 100 hours followed by 700°C for 40 hours. It is seen that if the temperature of the first heat treatment was higher than that of the second heat treatment, the Nb<sub>3</sub>Sn layer thickness increases of about 1 μm (Fig. 3b). If the second temperature was set at 750°C and held for 20 hours, the layer thickness increases of about 2.9 μm (Fig. 3d). However, the Nb<sub>3</sub>Sn-Nb flux does not result in any Nb<sub>3</sub>Sn layer ( $Y_{o Nb_3Sn-Nb} = 0$ ), since the amount of Sn at the boundary of first heat treatment was too low (Figs. 3c and e).



**Figure 3.** (a) Layer thickness of the first heat treatment (650°C/100 hours) (b) Layer thickness of the second heat treatment (Sn-Nb<sub>3</sub>Sn diffusion in 700°C/40 hours) and (c) Nb<sub>3</sub>Sn-Nb diffusion; (d) Layer thickness of the second heat treatment (Sn-Nb<sub>3</sub>Sn diffusion in 750°C/20 hours) and (e) Nb<sub>3</sub>Sn-Nb diffusion.



**Figure 4.** (a) Layer thickness of the first heat treatment (750°C/40 hours) (b) Layer thickness of the second heat treatment (Sn-Nb<sub>3</sub>Sn diffusion in 650°C/100 hours) (c) Nb<sub>3</sub>Sn-Nb diffusion.

Figure 4 shows the Nb<sub>3</sub>Sn layer formation if the temperature of second heat treatment was set to be lower than that of the first heat treatment. It is seen in Fig. 4b that the additional Nb<sub>3</sub>Sn thickness of about 0.2 μm was formed. The second flux towards Nb grain (Fig. 4c) is similar to that of Figs. 3c and 3e, where no Nb<sub>3</sub>Sn layer was obtained. It is clear that as the first temperature is lower than that of the second one, the less Sn solute will deplete into the Nb grain (2.1 μm), so that the degree of supersaturation remains high leading to further growth on the second heat treatment. On the contrary, as the first temperature is higher than the temperature of the second heat treatment, the large amount of Sn solute already depleted (4.5 μm), leading to less supersaturation degree and eventually less Nb<sub>3</sub>Sn layer formation on the second heat treatment. Similar results were reported that by increasing the second temperature heat treatment, the superconductivity properties of Nb<sub>3</sub>Sn increases considerably [11]. Nb<sub>3</sub>Sn layer thickness may affect the superconductivity properties (critical current I<sub>c</sub>). As the layer become thicker, the critical current I<sub>c</sub> will increase [2]. Apart from that, concentration of Sn at the GBs is the driving force of diffusion (C<sub>0</sub>). As the C<sub>0</sub> is higher, as described in equation (1), one would expect that the diffusion distance will increase, so as the C<sub>1</sub> leading further growth at the Nb<sub>3</sub>Sn -Nb boundary.

#### 4. Conclusion

In order to obtain the maximum Nb<sub>3</sub>Sn layer thickness, the second temperature of heat treatment must be set higher than the first temperature of heat treatment. The biggest layer thickness obtained was 2.9 μm for initial heat treatment at 650°C for 100 hours and second heat treatment at 750°C for 20 hours. The growth of the Nb<sub>3</sub>Sn at the Nb<sub>3</sub>Sn-Nb boundary depends largely on the concentration of Sn at the grain boundaries.

#### References

- [1] Dew-Hughes D. 1975. Superconducting A-15 compounds: A review. *Cryogenics*, 15:435-454.
- [2] Müller H., Schneider Th. 2008. Heat Treatment of Nb<sub>3</sub>Sn Conductors. *Cryogenics*, 48: 323-330.
- [3] Reddi B.V., Ray S., Raghavan V., and Narlikar A.V. 1978. Models for growth kinetics of A-15 compounds by solid state diffusion. *Phil. Magazine A*, Vol. 38:559-568.
- [4] Kaur I., Mishin Y., and Gust W. 1995. *Fundamentals of Grain and Interphase Boundary Diffusion*. Wiley Chichester.
- [5] Van Loo F.J.J., Rieck G.D. 1973. Diffusion in the titanium-aluminium system-II. Interdiffusion in the composition range between 25 and 100 at.% Ti. *Acta Metall.* 21:73-84.
- [6] Farrell H.H, Gilmer G.H, and Suenaga M. 1974. Grain Boundary Diffusion and Growth of Intermetallic Layers: Nb<sub>3</sub>Sn. *Journal of Applied Physics*, Vol 45 No.9: 4025-4035.
- [7] Fischer J.C. 1951. Calculation of diffusion penetration curves for surface and grain boundary diffusion. *Journal of Applied Physics*. 22 (1):74-77.
- [8] Whipple R.T.P. 1954. Concentration contours in grain boundary diffusion. *Phil. Magazine*. 45:1225-1237.
- [9] Barzi E., Mattafirri S. 2003. Nb<sub>3</sub>Sn Phase Growth and Superconducting Properties During Heat Treatment. *IEEE Trans. On Applied Superconductivity*, Vol 13, No.2: 3414-3417.
- [10] Muranishi Y., Kajihara M. 2005. Growth Behavior of Nb<sub>3</sub>Sn Layer during Reactive Diffusion between Cu-8,3 Sn Alloy and Nb. *Materials Science and Engineering A* 404: 33-41.
- [11] Rodrigues C.A, Machado J.P.B., and Rodrigues D. 2003. Development, Heat Treatment Optimization and Microstructural Characterization of Nb<sub>3</sub>Sn Superconductor Wire. *IEEE Trans. On Applied Superconductivity*, Vol.13, No. 2: 3426-3429.