1. Introduction: columnar grains in Nb$_3$Sn superconducting wire

- Nb$_3$Sn intermetallic compound is a processing material for high-field superconducting magnets with high critical temperature ($T_c = 23.2$ K), high critical magnetic field ($B_c = 45$ T), and high current density ($> 10^6$ A/cm$^2$) at 4.2 K.
- Nb$_3$Sn compound is usually utilized in wire form, but it is too brittle to be directly extruded into wire.
- Extrusion of Nb$_3$Sn layer in wire depends on the extrusion condition and extrusion temperature.
- Extrude a wire with Nb filaments inside a Sn-containing Cu matrix and then anneal (anneal process).
- Extrude a wire with Nb filaments and Sn core inside a Cu matrix and then anneal (intermediate process).

2. Development of Monte Carlo Potts model for interfacial reaction

- Place Nb$_3$Sn layer grows only toward the Pb phase since Sn diffuses much faster than Nb in Nb$_3$Sn (4).
- Annealing time is long (300–360 hours) to ensure grain growth within growing Nb$_3$Sn layers.
- Film, equilaxed Nb$_3$Sn grains are recommended when grain boundaries cause flux pinning (X, Y).
- Coarse columnar grains are usually observed in Nb$_3$Sn wire (P) and the detailed mechanism underlying such a columnar grain formation has not been clarified yet.

3. Literature review: full-scale Monte Carlo Potts grain growth model

- Algorithms of the MC Potts grain growth model (1).
  
  \begin{align*}
  P &= \frac{\exp(-\beta E)}{\sum_i \exp(-\beta E_i)}
  \end{align*}

  - Where $E$ is the energy difference (2).
  - Granular boundary mobility $\beta = \frac{1}{k_B T}$, where $k_B$ is Boltzmann constant.
  - Activation energy of grain growth in the real world
  \begin{align*}
  \frac{dG}{dt} &= \frac{1}{\Delta_t} \sum_i \frac{dA_i}{dt} = \frac{1}{\Delta_t} \sum_i \left( \frac{1}{\tau} \right)
  \end{align*}

    - $\tau$ is the transition time (0).
    - Activation energy of grain growth in the real world

4. Simulation of Nb$_3$Sn layer growth reaction

- Annealing time is long (300–360 hours) to ensure grain growth within growing Nb$_3$Sn layers.
- Film, equilaxed Nb$_3$Sn grains are recommended when grain boundaries cause flux pinning (X, Y).
- Coarse columnar grains are usually observed in Nb$_3$Sn wire (P) and the detailed mechanism underlying such a columnar grain formation has not been clarified yet.

Conclusion

A novel Monte Carlo Potts model for interfacial reactions is developed. By utilizing thermodynamic information, the model well reproduces the diffusional growth of the Nb$_3$Sn layer and accompanying grain evolution. The fundamental reason for the formation of coarse columnar grains in the growing Nb$_3$Sn layer is the decrease in the thermodynamic driving force of nucleation, due to the insufficient accumulation of Sn at the reaction front (Nb$_3$Sn/Sn interface).

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References