

Define a Variable Temperature Range in a tdb File

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June 19, 2020

Abstract

How to define a magnetic model with a variable temperature limit in a tdb file?

Problem

How to implement a magnetic model parameter

$$f = \begin{cases} \sqrt{1 - \frac{T}{T_c}} & \text{for } T \leq T_c \\ 0 & \text{for } T > T_c \end{cases} \quad (1)$$

in a tdb file?

Solution

Using a `sign` function. `sign` is defined as

$$\text{sign}(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x = 0 \\ -1 & \text{for } x < 0 \end{cases} \quad (3)$$

$$\text{sign}(x) = \begin{cases} 0 & \text{for } x = 0 \end{cases} \quad (4)$$

$$\text{sign}(x) = \begin{cases} -1 & \text{for } x < 0 \end{cases} \quad (5)$$

The magnetic model parameter f can be implemented in a tdb file in following sentences.

```
Function TC_BCC 298.15 Tc(@BCC_A2); 6000 N !
Function term_Tc 298.15 1-T/TC_BCC; 6000 N !
Function p_Tc 298.15 0.5*(sign(term_Tc)+1)*term_Tc; 6000 N !
Property f 298.15 sqrt(p_Tc); 6000 N !
```