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Research on Lattice Entropy Change of Heusler Alloy Ni_2MnSb

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Abstract

In the magnetic properties of Hasler alloy, magnetocaloric effect is of great significance. In this paper, the change of Ni_2MnSb lattice entropy is studied by Debye model, the change law of Ni_2MnSb lattice entropy with respect to temperature is analyzed, and the relationship between magnetic entropy and lattice entropy in entropy change is compared. It is found that the change of magnetic entropy of Ni_2MnSb at 270k is less than that of lattice entropy.

Keywords

Research , Lattice Entropy , Heusler Alloy Ni_2MnSb.

1. Introduction

Heusler alloy has both ferromagnetic transformation and thermoelastic martensitic transformation, and rich magnetic state and special properties of variable magnetic transformation driven by magnetic field, especially the variable magnetic shape memory effect, magnetic card effect and magnetoresistance effect in this process, which have broad application prospects [1-3]. The concentrated research on Heusler alloy in the world began in 1980s. The thermoelastic martensitic transformation, shape memory effect, magnetic origin and crystal structure of Heusler alloy have been studied in a series [4-7]. By changing the stoichiometric ratio of elements in Ni-Mn-Ga alloy, the martensitic transformation temperature and Curie temperature of the material change regularly, and the magnetically induced strain of single crystal also changes accordingly. In recent years, researchers have introduced a proper amount of fourth component (such as Cu, Fe) into Ni-Mn-X (X=In, Sn, Sb) alloys to replace Ni atoms or Mn atoms in the alloys, so as to improve the ferromagnetic exchange in the parent phase and further increase the magnetic difference between the parent phase and martensite phase. Therefore, the structure and magnetic properties of quaternary Heusler alloy samples have been analyzed. The researchers found that with the increase of the content of the fourth component, the properties and structure of the materials changed. This shows that the composition in Heusler alloy has a significant effect on the crystal structure and magnetic properties [8-10].

Magnetocaloric effect is of great significance among the magnetic properties of Heusler alloy, which refers to the exothermic/endothermic phenomenon of materials when the external magnetic field strength changes. Because of its high energy conversion efficiency, the magnetocaloric effect of materials has attracted the attention of many researchers. The research shows that the magnetocaloric effect of Heusler alloy is very significant, but the mechanism of magnetocaloric effect is still unclear. In the related research of S. M. Podgornykh et al., the relationship between lattice and heat capacity is studied by theoretical calculation, and it is found that crystal structure has great contribution to heat capacity [12]. According to the research of H. Oesterreicher and F. T. Parker [11], the entropy change caused by magnetic field is caused by three parts: Electron entropy, lattice entropy and magnetic entropy. However, most of the researches on magnetocaloric effect of Heusler alloy are focused on experiments, and the contribution degree of electronic structure, crystal structure and magnetism to total entropy change is still unclear.

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The lattice entropy of Ni_2MnSb is studied by using Debye model, and compared with the experimental data. The variation law of lattice entropy with respect to temperature is analyzed, and the relationship between magnetic entropy and lattice entropy in entropy change is compared.

2. Experimental Methods

In 1912, Debye put forward an atomic vibration model for calculating the heat capacity of solids-Debye model. Based on Einstein's model, Debye's model holds that heat capacity should be the sum of atomic vibrations at various frequencies, which obtains a new equation of solid heat capacity which accords with experimental results.

According to the research of H. Oesterreicher and F. T. Parker, the equation for calculating lattice entropy of solid crystal is as follows

$$S_L = mR\left[-3ln(1-e)^{-\theta_D/T} + 4D\left(\frac{\theta}{T}\right)\right] \text{[11]} \tag{1}$$

R is the gas constant, θ_D is the Debye temperature, and D(x) can be obtained from the above research as

$$D(x) = 1.000 - 0.375x + 0.050X^2 - 0.0011x^3 \text{ [11]}$$

In a form convenient for calculation, it can be expressed as

$$S_L = R\left[-3ln\left(1-e^{T_D/T}\right) + 12\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^3dx}{e^x-1}\right] \tag{2}$$

R is the gas constant and T_D is the Debye temperature.

According to the experimental results of S.M. Podgornykh et al., the Debye temperature of Ni_2MnSb is 222K [12].

3. Experimental Results and Analysis

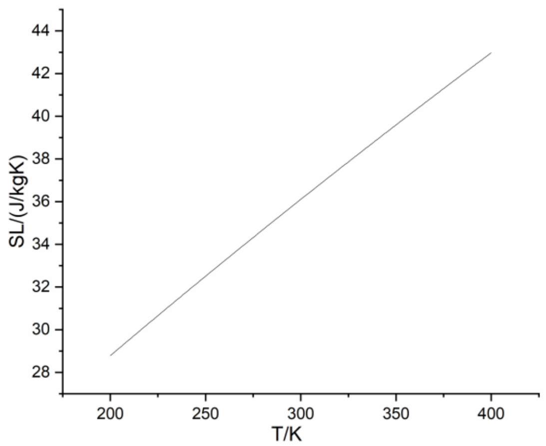

Figure 1 Graph of Ni2MnSb lattice entropy changing with temperature

Figure 1 is the curve of lattice entropy of Ni_2MnSb alloy with temperature in the temperature range from 200K to 400K calculated by Debye model. It can be seen from Figure 1 that the lattice entropy of Ni_2MnSb alloy increases with the increase of temperature. Further analysis shows that the relationship between lattice entropy and temperature of Ni_2MnSb alloy can be fitted by polynomial, and the fitting equation is as follows:

$$y = \text{-}2E\text{-}05x^2 + 0.0844x + 12.805$$

Further analysis shows that the lattice entropy of Ni_2MnSb alloy increases by 49.6% from 200K to 400K. The lattice entropy of Ni_2MnSb alloy is caused by the thermal vibration of atoms. According to Debye's model, the thermal changes of solids are caused by the thermal vibration changes of atoms at the microscopic level. When the temperature rises, the thermal motion of atoms accelerates. However, atoms are bound by crystal fields at the same time. When the thermal vibration of atoms is strengthened, the interaction between adjacent atoms becomes stronger. This, in turn, binds the thermal vibration.

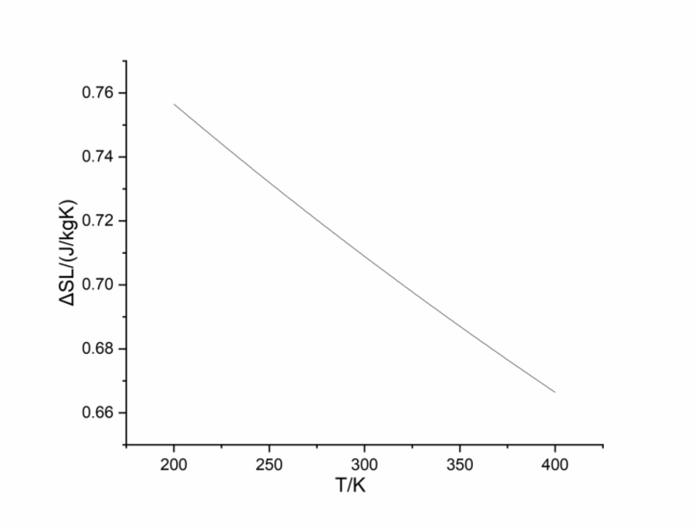

Figure 2 Lattice entropy change rate of Ni_2MnSb

Figure 2 is the curve of lattice entropy change rate of Ni_2MnSb alloy with temperature from 200K to 400K. It can be seen from Figure 2 that the lattice entropy change rate of Ni_2MnSb alloy decreases with the increase of temperature. Further analysis shows that the relationship between lattice entropy and temperature of Ni_2MnSb alloy can be fitted by polynomial, and the polynomial obtained by fitting is as follows:

$$y = 3E\text{-}07x^2 - 0.0006x + 0.867$$

There is no experimental report on magnetic entropy change of Ni_2MnSb alloy in literature. Therefore, the magnetic entropy change data of $Ni_{50}Mn_{37}Sb_{13}$ alloy are used for comparison in this paper. According to the research of Mahmud Khan et al., it can be known that the magnetic entropy of $Ni_{50}Mn_{37}Sb_{13}$ at 270K changes to 10.77J/kgK at 5T magnetic field and 3.49J/kgK at 2T magnetic field, both of which are smaller than the lattice entropy change of Ni_2MnSb at 270K (33.96 J/kgK) [13]. Studies in the literature show that only ferromagnetic exchange exists in Ni_2MnSb alloy, and antiferromagnetic exchange is newly formed in Ni2MnSb alloy with the increase of Mn content. With the increase of Mn content, the saturation magnetic moment of the alloy decreases. When the external magnetic field strength is low (such as 2T), the response of antiferromagnetic exchange to external magnetic field is more obvious, and only when the magnetic field strength is high (such as 5T), the response of ferromagnetic exchange to external magnetic field is more obvious. The magnetic entropy change of $Ni_{50}Mn_{37}Sb_{13}$ alloy is larger than that of Ni_2MnSb alloy in small magnetic field. Therefore, the change of magnetic entropy of Ni_2MnSb at 270K is less than that of lattice entropy.

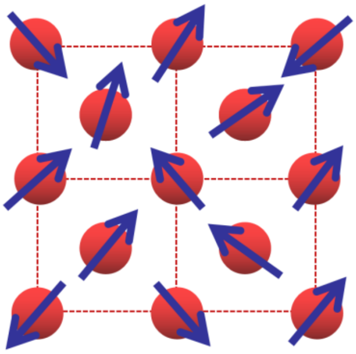

Figure 3 Structural diagram of Ni_2MnSb alloy

Figure 3 is a schematic diagram of crystal structure and magnetic structure of Ni_2MnSb alloy. As shown in Figure 3, the interaction between atoms in Ni_2MnSb alloy constitutes the lattice, and the magnetic moment carried by atoms constitutes the magnetism of the alloy. When the interaction between atoms changes, the magnetism will also change. With the increase of temperature, the magnetism of atoms changes when the thermal vibration increases. When an external magnetic field is applied to the alloy, the magnetocaloric effect of the alloy includes the contribution of crystal and magnetism, which is due to the strong coupling between structure and magnetism in the alloy. Therefore, the contribution of lattice entropy should be considered in the study of magnetocaloric effect of this alloy.

4. Conclusion

In this paper, the change of lattice entropy in Ni_2MnSb alloy is studied by Debye model. Compared with the relevant experimental data, the change law of lattice entropy with respect to temperature is analyzed, and the relationship between magnetic entropy and lattice entropy in entropy change is compared. It is found that the magnetic entropy change of Ni_2MnSb alloy at 270K is less than that of Ni_2MnSb alloy at 270K.

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