Micro-structure Parameter Optimization Design of Short-fiber/ whisker Reinforced Composite

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Abstract: The influence on the stiffness modulus of composites exerted by the volume fraction of reinforcers, aspect ratio, the modulus ratio of the whisker to the matrix, the effect of reinforcers orientation and heat treatment state is discussed, the quantificational relations between micro-structure parameters of the short-fiber/whisker reinforced metal matrix composite and its macro mechanical properties are built, and an optimal design method of micro-structure parameters about original isotropy and singularity tropism distribution of the whisker reinforced metal matrix composite is developed. Typical optimal design examples concerning the micro-structure parameter of this kind of material are presented.

Key words: whisker reinforced composite; micro-structure parameter; optimal design

晶须增强金属基复合材料微结构参数优化设计. 李敏, 刘秋云, 刘晓宇, 梁乃刚. 中国航空学报(英文版). 2001, 14(3): 147- 154.

摘　要: 讨论了增强体体积比、长径比、基体与增强体的模量比以及增强体取向分布、基体的热处理状态对复合材料刚度模量的影响, 建立了晶须增强金属基复合材料微结构参数与宏观力学性能间的定量关系, 探索了晶须增强金属基复合材料微结构参数优化设计方法, 给出了该材料微结构参数优化设计的典型算例。

关键词: 短纤维/晶须增强复合材料; 刚度预测; 微结构参数优化
文章编号: 1000-9361(2001)03-0147-08　中图分类号: V214.8; V257　文献标识码: A

The composite property has a close relation with the volume and micro-structure parameters of reinforcers. How to derive the composite macro mechanical property from micro-structure physical and geometrical parameters, and, in return, how to do an optimal design for the micro-structure parameters according to mechanical properties of composites; both problems are of great concern but are not solved very well[1,2].

In recent years, the meso-mechanics has been applied to composite research and the relation between the composite material micro-structure and macro mechanical property has been built up[2-4]. For example, for a small aspect ratio and low volume fraction, the elastic property of the whisker or grain reinforced composite can be perfectly predicted by Eshelby equivalent inclusion method[4,5]. A modified shear lag model has been employed for property prediction of the short fiber reinforced composite with higher aspect ratio and low volume fraction[6-8]. But for the composite material used in practical engineering with high volume fraction reinforced, the property prediction is difficult[9]. The prediction theory concerning the mechanical property and optimal design of the composite material can provide theoretical foundation for reasonable material design and utilization, and promote wider application of composites. All these questions are crying out for solution.

The influence of tropism distributing of short fiber/whisker on the material macro property was calculated in Ref. [10], in which the space location distributive randomicity of short

Received date: 2001-02-14; Revision received date: 2001-04-26
Foundation items: National Nature Science Foundation of China(19872065, 19732060), Chinese Academy of Sciences Foundation(KGCX1-11) and Post Doctor Science Foundation of China
Article URL: http://www.hkxb.net.cn/cja/2001/03/0147/

fiber/whisker and the strain distributive detail in the end of reinforcers were neglected, and stiffness tensor expression of the composite was derived by introducing a matrix and reinforcers' deformed availability coefficient and tropism distributing density function of reinforcers; with this function the stiffness tensor of the composite in engineering can be predicted in the condition of arbitrarily tropism distributing reinforcers and arbitrarily deformed condition. The upper limit and lower limit of the composite material stiffness correspond to an equal strain model (mixed theorem) and equal stress model respectively; arbitrary values of the stiffness module from the upper limit to low limit correspond to a set of specific availability coefficients, so that the predictive precision can be guaranteed[11].

Based upon a prediction theory[10], the quantificational relations between the micro-structure parameter of the whisker reinforced metal matrix and macro mechanical property are built in this paper. Aimed at composite materials with original isotropy (random tropism distributing reinforcers) or singularity tropism, with given material macro mechanical property, an optimal design of micro-structure parameters was implemented.

1 Deformed Statistical Character and Strain Energy of Reinforcers and Matrix

The reinforcer deformation characteristic parameter λ_f is defined as the ratio of the average root-mean-square strain of whiskers to the macro-linear strain along the same direction, written as

$$\lambda_f = \frac{\bar{\epsilon}_f}{\epsilon} \tag{1}$$

where $\bar{\epsilon}_f$ is the root-mean-square strain of reinforces oriented in l direction, as shown in Fig. 1, and ϵ, the macro-linear strain along the same direction.

It can be proved that on condition of elastic

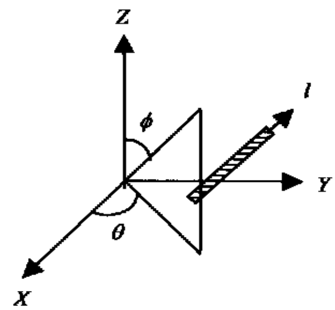

Fig. 1 Schematic diagram of whisker orientation

deformation, $\bar{\lambda}_f$ depends on the volume fraction of reinforcers, aspect ratio and modulus ratio of the reinforcers to the matrix only, and it is independent of macro deformation. $\bar{\lambda}_f$ is an intrinsic characteristic parameter of the composite and can be expressed as[10]

$$\lambda_f = f\left(\frac{E_m}{E_f}, \frac{L}{d}, V_f\right) \tag{2}$$

where V_f is the volume fraction of whiskers in l direction; $\bar{L}$ and $\bar{d}$ are the average length and diameter of reinforces respectively; E_f and E_m are the elastic moduli of whisker and matrix respectively.

From Ref. [10], the strain energy in unit volume of composite is

$$W_c = \frac{1}{2}\lambda_m^2 V_m S_{(m)ijrs}\epsilon_{ij}\epsilon_{rs} + \frac{1}{2}E_f\epsilon_{ij}\epsilon_{rs} \times \int_0^{\pi/2}\sin\phi\int_0^{2\pi}\lambda_f^2(\theta,\phi)\rho(\theta,\phi)n_i n_j n_r n_s \mathrm{d}\theta\mathrm{d}\phi \tag{3}$$

where the definitions of ϕ and θ are shown in Fig. 1; $\rho(\theta,\phi)$ is the reinforcer orientation density function; $n_i (i = 1, 2, 3)$ is the directional consines of a unit vector, and satisfies

$$\begin{cases} n_1 = \sin\phi\cos\theta \\ n_2 = \sin\phi\sin\theta \\ n_3 = \cos\phi \end{cases} \tag{4}$$

λ_m is an intrinsic characteristic parameter of the matrix; for composites with singular direction distributing or random tropism reinforcers, there exists

$$\lambda_m V_m + \lambda_f V_f = 1$$

i.e.

$$\lambda_m = \frac{1 - V_f\lambda_f}{V_m} \tag{5}$$

The stiffness tensor of the composite can be obtained by performing twice differentials to Eq.

(3), that is

$$S_{(c)ijrs} = \lambda_m^2 V_m S_{(m)ijrs} + E_f \int_0^{\pi/2} \sin\phi \int_0^{2\pi} \lambda_f^2(\theta,\phi)\rho(\theta,\phi) n_i n_j n_r n_s \mathrm{d}\theta \mathrm{d}\phi \quad (6)$$

Specially, when reinforcers randomly oriented in X-Y plane, the simple expression for the stiffness tensor can be written as

$$S_{(c)ijrs} = \lambda_m^2 V_m S_{(m)ijrs} + E_f \int_0^{\pi} \lambda_f^2(\theta)\rho(\theta) n_i n_j n_r n_s \mathrm{d}\theta \quad (7)$$

where θ is the angle of whisker orientation and X axis.

After the micro-structure physical and geometrical parameters of the composite and reinforcer orientation density function are known, by Eqs. (6) and (7), the stiffness of the composite can be predicted. Based on the stiffness prediction theory mentioned above and knowing the stiffness tensor of the composite, the structure parameter of the composite can be optimized.

2 The Influence of Micro-structure Parameter of Material on the Stiffness of Composite

The optimal design for micro-structure parameters of the composite includes physical and geometrical parameter optimization. The process of selecting material is the optimal process for physical parameters. When the reinforcer and matrix are fixed, the physical parameters can be obtained uniquely. For special composites, the same macro property can be achieved by different combinations of geometrical parameters, so the process, deciding the volume fraction of reinforcers, aspect ratio, oriented distribution and heat treatment state, is the optimal process for geometrical parameters of the composite.

Optimal design is based on building the quantitative relationship of micro-structure physical and geometrical parameters of the composite to macro mechanical properties, so first in the following, the influence of the geometrical parameter on the stiffness of the composite is analyzed. It should be noted that because the interface of the whisker reinforced metal matrix composite is conjunctive well, belonging to a strong interface, the influence of the conjunct intensity of the interface on the macro property is neglected in this paper.

2.1 The influence of the volume fraction of reinforcers, aspect ratio and modulus ratio of reinforcers on the stiffness of composite

It can be known from Eqs. (6) and (7) that all parameters which influence λ_f must do work to the stiffness of the composite. According to Eq. (2), it can be known that the volume fraction of reinforcers, aspect ratio and modulus ratio of the reinforcers to the matrix should influence λ_f. By using the 2-D network model[12], the influences of these aforementioned material parameters on λ_f were investigated; the simulative results were shown in Fig. 2. By using the least square method, the regression formula of λ_f, in the range of linear elastic deformation, can be expressed as[13]

$$\lambda_f^{(e)} = 1.4(0.94 + 0.3V_f)\left(\frac{E_m}{E_f}\right)^{\left(0.84 - 0.03\frac{L}{d}\right)} \quad (8)$$

$(V_f: 5\% - 40\%, L/d: 3 - 15, E_m/E_f: 0 - 1/3)$

where L and d are the average length and diameter of reinforces respectively. The aspect ratio of reinforcers means L/d, and the same hereinafter. In this analysis, the modulus of the reinforcer is assumed higher than that of the matrix, the modulus ratio of matrix to reinforcer ranging between 0 and 1/3. Those aforementioned material parameters have a linear influence on λ_f. In Fig. 2, the comparison of two results predicted by regression formula Eq. (8) and network model respectively, λ_f, changing with L/d and E_m/E_f, is provided, and it can be seen that the two results agree well.

Effective load undertaken by reinforcers would increase with the increase of the volume fraction and aspect ratio, so λ_f would increase and the stiffness of the composite would also increase. λ_f increases with the increase of moduli of matrix modulus to reinforcers modulus, which means that the closer the modulus of the matrix is to that of the reinforcer, the more easily the performance potential of those two would be brought into play sufficiently.

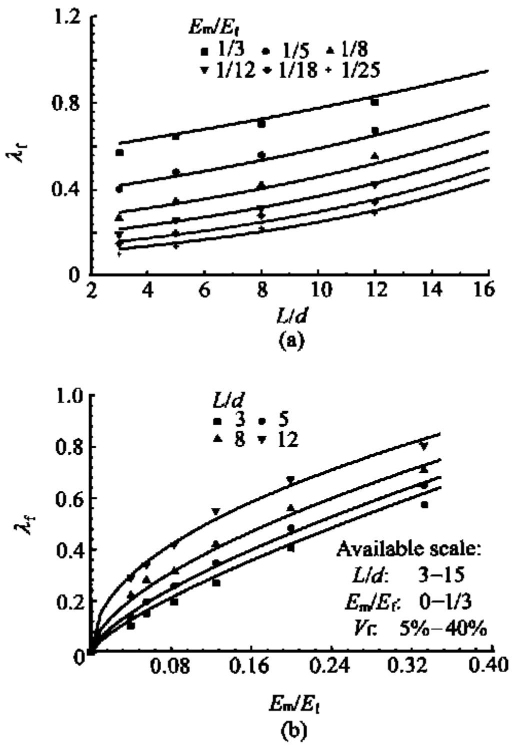

Fig. 2 The curve of λ_f versus L/d and E_m/E_f

2.2 The influence of tropism distributing of reinforcers on stiffness of composite

The tropism distributing of reinforcers can be changed by mature technics in engineering, the quantitative analysis of the influence of tropism distributing of reinforcers on the stiffness of the composite has an important practical significance.

When reinforcers are unidirectionally oriented, the orientation density function can be expressed by a unit pulse function, *i.e.* $\rho(\theta, \phi) = V_f\delta(0, \pi/2)$. Provided that reinforcers are oriented in X-axis direction, from Eq. (6), it is known that the stiffness modulus of the composite in X-axis direction is as follows

$$S^{(0)}_{(c)1111} = \lambda_m^2 V_m S_{(m)1111} + \lambda_f^2 V_f E_f \quad (9)$$

If $\lambda_f = \lambda_m = 1$, Eq. (9) is changed into the famous mix law, which can provide the maximum value (upper limits) of the stiffness modulus of the composite

When whiskers oriented randomly in 3-D space, $\rho(\theta, \phi) = V_f/2\pi$, from Eq. (6) it can be yielded that

$$S^{(p3)}_{(c)1111} = \lambda_m^2 V_m S_{(m)1111} + \lambda_f^2 V_f E_f \frac{1}{2\pi}\times \int_0^{\pi/2}\sin^5\phi\int_0^{2\pi}\cos^4\theta\,d\theta\,d\phi = \lambda_m^2 V_m S_{(m)1111} + \frac{1}{5}\lambda_f^2 V_f E_f \quad (10)$$

Comparing Eq. (9) and Eq. (10), one can find that the contribution of reinforcers to the stiffness of the composite, when whiskers oriented randomly, is only 1/5 as that when reinforcers are unidirectionally oriented. So to adjust the tropism of reinforcers is an effective method for providing the stiffness modulus of the composite.

For instance, aimed at SiCw/Al whisker reinforced metal matrix composite, the influence of the tropism distributing of reinforcers on the stiffness of the composite is quantitatively analyzed. The stiffness modulus of the matrix and reinforcer are 70 GPa and 450 GPa; the volume fraction of reinforcers is 40%; the aspect ratio is 10. By Eqs. (8) and (3), λ_f and λ_m are calculated out to be 0.54 and 1.3 respectively. According to Eq. (9), the stiffness modulus of the composite is 130.5 GPa when reinforcers are unidirectionally oriented. Where the first item in Eq. (9), *i.e.* the contribution to the stiffness of the composite about the matrix is 78GPa, the second item, *i.e.* that about (of) reinforcers is 52.5 GPa. According to Eq. (10), the stiffness modulus of the composite is 88.5 GPa, the contribution of matrix and reinforcers are 78 GPa and 10.5 GPa, and thus the contribution of reinforcers just takes 12%. So the stiffness of the composite would not increase remarkably with reinforcers leading in the metal matrix. In order to achieve a higher modulus, the reinforcers must arrange directionally.

The methods to adjust tropism of reinforcers used in engineering practice are heat extrusion, forge, rolling and so on. For instance, with heat extrusion, the directional arrangement level of reinforcers is controlled by the ratio of extrusion. The higher the ratio, the more remarkable the effect of directional arrangement. But the aspect ratio of reinforcers would decrease with the ratio of extrusion increasing, so the effect of reinforcement would be weaker than before. It is obvious that the ratio of extrusion is a parameter needed to be optimized in engineering practice. The relationship between the ratio of extrusion and tropism of reinforcers is shown in Fig. 3. It can be seen that when the ratio of extrusion reaches 16, the tropism of reinforcers is very close to unidirectional arrangement.

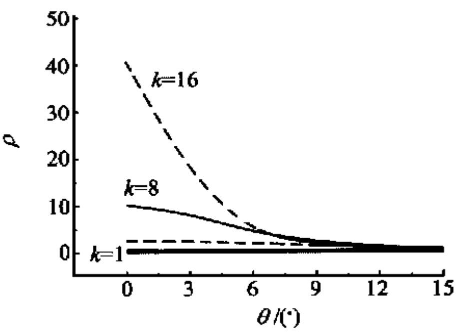

Fig. 3 The ratio of extrusion and tropism of reinforcers

2. 3 The influence of matrix on mechanical properties of metal matrix composite

The earlier research indicated[15] that the dislocation density of the matrix is between 10^{13} – 10^{14} m^{-2} in metal matrix composites, 10– 100 times that in the original matrix metal; meanwhile, the crystal size in the matrix changes into a smaller size evidently with introducing reinforcers. The matrix material in the composite fills in the gap between the reinforcers mainly, the size of matrix crystal matches with the gap between reinforcers. For instance, aimed at ScWu/Al whisker reinforced composite, the gap between reinforcers matched with the diameter of reinforcers, is about 1μm, but the size of crystal in the matrix material is above 10μm. Hence it is obvious that the matrix material in the composite differs from the pure matrix material. If this difference is ignored, the theoretical prediction of properties will be lower[16].

In addition, for the metal material that heat treatment can be applied to, the mechanical properties can be improved by succedent heat treatment. For instance, aimed at whisker reinforced aluminium matrix composite, the matrix material always is the forging aluminium alloy or casting aluminium alloy. Not only has this alloy favorable fluidity and moulding, but also the mechanical properties can be improved by heat treatment.

The solution treatment and ageing treatment are popular methods for heat treatment. The purpose of solution treatment is to obtain metastable supersaturation, and the purpose of ageing treatment is to let new phase precipitate. Because the precipitative phase sometimes is not a balance phase in the phase picture, but a metastable phase or congeries of solute atoms, the intensity and rigidity can be improved remarkably by this way.

The analysis above indicates that the difference between the matrix material in the composite and pure matrix alloy should be considered for predicating reasonably mechanical properties of composites.

3 Optimal Design for Whisker/Short Fiber Reinforced Metal Matrix Composite

According to the quantitative relationship derived above between the physical and geometric parameters of micro structure in the composite and macro mechanical properties, the micro structure parameters in the composite can be chosen when the stiffness tensor is known.

3. 1 The estimation of micro structure parameters

In order to do optimal design for the micro structure of the matrix and reinforcers, the upper limit and lower limit of the stiffness in the composite should be calculated out first using limits of these parameters, and it should be made sure that the stiffness value is in between the upper limit and lower limit.

For unidirectionally whisker reinforced composites, when $\lambda_f = \dfrac{S_{(m)1111}}{S_{(m)1111}V_f + E_f V_m}$, $\lambda_m = \dfrac{E_f}{S_{(m)1111}V_f + E_f V_m}$, the stiffness modulus in Eq. (9) takes a minimum. When $\lambda_f = \lambda_m = 1 (0 < \lambda_f \leq 1)$, the stiffness modulus takes a maximum, expressed as[11]

$$S_{(c)1111} = V_m S_{(m)1111} + V_f E_f \tag{11}$$

There must exist a specified λ_f and λ_m corresponding to a stiffness value which is between the upper limit and lower limit. That means there must be a group of or some sets of physical and geometric parameters of micro structure that can satisfy the stiffness need of the composite.

3.2 The typical examples for optimal design of composite

Example 1. The stiffness modulus of the composite is not allowed to be below 300GPa.

The matrix and reinforcers are chosen first, so that the stiffness moduli of the matrix and reinforcers are confirmed. In this example the reinforcers are chosen as SiC whisker and the matrix material is chosen as Al or Ti alloy. Their stiffness moduli are 480GPa, 70GPa and 120GPa respectively. As the required stiffness of the composite is far greater than the one of the matrix, the volume fraction of reinforcers takes the upper limit, *i.e.* 40%. From Eq. (12), the upper limit values of the stiffness modulus in the composite are 238GPa and 264GPa respectively, which can not reach the required value, 300GPa, so a matrix and reinforcers having higher modulus were selected.

The carbon fiber whose stiffness modulus is 800GPa is chosen as the reinforcer and the Al alloy as matrix. The volume fraction takes the upper limit, 40%. From Eq. (11), the upper limit value of the stiffness is obtained, 362GPa, and greater than the required value 300GPa. According to the above analysis, the stiffness modulus in some direction of this kind of composite may reach 300GPa. The aspect ratio of reinforcers takes 15; according to Eqs. (3) and (8) λ_f and λ_m are 0.574 and 1.284 respectively; according to Eq. (9) the stiffness of the composite is 181.6GPa.

In the above example, though the required stiffness of the composite is located between the upper limit and lower limit, the short fiber reinforced composite with stiffness modulus greater than 300GPa, can not be obtained in engineering practice because of the limit of manufacture technique. For obtaining the composite that possesses higher stiffness modulus, better property reinforcers and new manufacture technique must be developed to increase the volume fraction of reinforcers and the aspect ratio of reinforcers.

By the way, the stiffness modulus of the matrix in the composite is 1.1 times greater than the one in the pure matrix alloy as the difference being considered between them.

Example 2. The stiffness modulus in a certain direction is required to be 90, 95, 100, 105, 110, 115 and 120GPa above.

The stiffness modulus of the composite above is as 1.5– 2 times as that one of Al alloy. So Al alloy is chosen as the matrix and SiCw/Al whisker as the reinforcer; their stiffness moduli are 70GPa and 450Gpa respectively. Only the stiffness modulus in one direction is required, so the tropism distributing of reinforcers is unidirectionally. The volume fraction takes the lower limit 5%. $\lambda_f = \dfrac{S_{(m)1111}}{S_{(m)1111}V_f + E_f V_m}$, $\lambda_m = \dfrac{E_f}{S_{(m)1111}V_f + E_f V_m}$, according to Eq. (9) the lower limit of the stiffness modulus is 80GPa. If the volume fraction takes the upper limit 40% and $\lambda_f = \lambda_m = 1$, according to Eq. (11) the upper limit of the stiffness modulus is 226GPa. Because the required modulus is between the upper limit and lower limit, the specific λ_f and λ_m are corresponding to the required modulus value.

In the following, for instance, with the stiffness modulus of the composite being

100GPa, the optimal designing process for geometric parameters is shown.

The stiffness moduli of the matrix and reinforcer are 70GPa and 450GPa respectively. Substituting Eq. (5) and the material stiffness modulus into Eq. (9) yields

$$(1 - \lambda_f V_f)^2 \frac{70 \times 1.1}{(1 - V_f)} + 450 V_f \lambda_f^2 = 100 \quad (12)$$

The unknown variable in Eq. (12) is the volume fraction of reinforcers V_f and λ_f. If V_f is fixed, λ_f is fixed on exclusively. This means if V_f takes any value between 5%–40%, there will be a specific λ_f corresponding to this V_f. Fixing the volume fraction of reinforcers, the equation about λ_f can be obtained

$$(V_f E_f + V_f^2 E_m/(1 - V_f))\lambda_f^2 - 2V_f E_m/(1 - V_f)\lambda_f + E_m/(1 - V_f) - E_c = 0 \quad (13)$$

The variational range of the volume fraction of reinforcers is 5%～40%. If $V_f = 20\%$, λ_f is 0.49.

According to Eq. (8),

$$L/d = 28 - (\ln\lambda_f - \ln 1.4 - \ln(0.94 - 0.3V_f))/(0.03\ln(E_m/E_f)) \quad (14)$$

Substituting V_f, λ_f, E_m, E_f into Eq. (14), the aspect ratio is obtained as 8.2, which is in between the range 3–15 being in the variational range of the aspect ratio.

When the volume fraction of reinforcers changes, the analysis for Eqs. (13) and (14) will be repeated, so that the corresponding λ_f and L/d can be obtained. Maybe many combinations could reach the same property required; all feasible combinations satisfying the stiffness requirement and design process are shown in Fig. 4.

(1) If the volume fraction of reinforcers is known, the process calculating the aspect ratio is shown as arrowhead 1 in Fig. 4. λ_f can be obtained from Eq. (13), and L/d can be obtained from Eq. (14).

(2) The aspect ratio of reinforcers can be fixed first, then the volume fraction can be calculated. The process is shown as arrowhead 2 in Fig. 4. According to Eqs. (13) and (14), V_f and λ_f can be obtained.

(3) After the aspect ratio and volume fraction of reinforcers are fixed, the stiffness modulus of the composite could be fixed on exclusively; this process is shown as arrowhead 3 in Fig. 4.

In engineering practice, according to the requirement for the stiffness modulus of the composite, the corresponding variational curve of micro structure parameters can be drawn similarly with Fig. 4, so as to built a quantitative relation between the micro structure parameter and material macro property, and then the optimal design to(for) micro structure parameters of the composite can be realized.

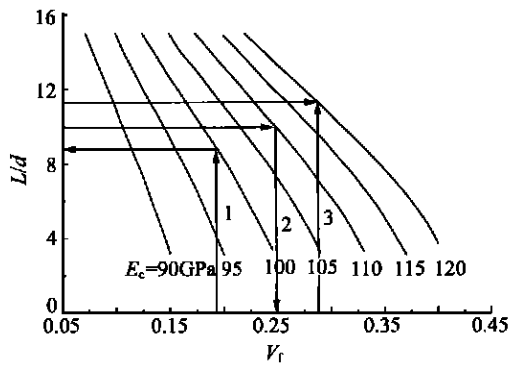

Fig. 4 The effectiveness of micro-structure parameter to properties of composite

4 Conclusions

(1) For predicting mechanical properties of the composite reasonably, the difference between the matrix in the composite and pure matrix alloy should be considered.

(2) When whiskers are oriented randomly, the reinforcement effect is only 1/5 as that when reinforcers are unidirectionally oriented. The stiffness modulus of the composite does not increase remarkably following the increase in the volume fraction of reinforcers.

(3) Based on the prediction theory built in this paper, the optimal design of micro structure physical and geometrical parameters of the composite can be realized.

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