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论文

α_2-Ti-25Al-*x*Nb合金力学性质的第一原理计算

曾宪波,彭平

湖南大学材料科学与工程学院, 长沙 410082

摘要:

采用第一原理赝势平面波方法计算了$D0_{19}$结构的α_2-Ti-25Al-*x*Nb(*x*=0-12, 原子分数, %) 晶体的弹性模量(*B*, *G*和*E*) 和抗拉强度 (σ_b), 并利用Cauchy压力(c_{12}-c_{44})与*G*/*B*比值表征和评判了不同浓度Nb合金化时α_2-Ti-25Al-*x*Nb合金的韧脆化倾向. 结果表明: 在 *x*=2-12时, α_2-Ti-25Al-*x*Nb晶体的抗拉强度 (σ_b)与α_2相合金的弹性模量(*B*, *E*和*G*)随x增加而增大; 在*x*=0-6时, α_2-Ti-25Al-*x*Nb合金脆性有一定改善, 且*x*值越大韧化效果越好; 但在*x*=7-9 时, 相对于α_2-Ti_3Al, 合金脆性不但没有得到弱化, 反而随*x*增加而加剧; 随后, 当*x*进一步增大时, 合金脆性又随*x*增加再次得到改善, 至*x*=12时, α_2-Ti-25Al-*x*Nb合金的韧化效果最好. 通过电子态密度 (DOS) 和投影电子态密度 (PDOS)等电子结构的分析, 初步解释了Nb的这种强化与韧化作用.

关键词: α_2-Ti_3Al Nb合金化 力学性质 第一原理计算-Ti_3Al Nb合金化 力学性质 第一原理计算

CALCULATION OF MECHANICAL PROPERTIES OF α_2-Ti-25Al-*x*Nb ALLOYS BY FIRST-PRINCIPLES

ZENG Xianbo, PENG Ping

School of Materials Science and Engineering, Hunan University, Changsha 410082

Abstract:

Intermetallic alloys based on Ti_3Al are potential high-temperature structural materials due to their low density, high specific strength, excellent creep behavior and good oxidation resistance, but their application has been hampered by the low room--temperature ductility and ambient brittleness. Numerous experiments have shown Nb is most effective additive to improve their ductility and toughness at low temperature, but the influence of Nb content on the mechanical properties of Ti_3Al-based alloys has not been understood. In this work, using the first-principles pseudo--potential plane wave method, ultimate tensile strength σ_b of α_2-Ti-25Al-*x*Nb (*x*=0-12, atomic fraction, %) single crystal with $D0_{19}$ structure and bulk modulus *B*, Young's modulus *E* as well as shear modulus *G* of α_2-Ti-25Al-*x*Nb polycrystalline alloys have been calculated, and their ductile/brittle behavior is characterized and assessed by the Cauchy pressure (c_{12}-c_{44}) and the *G*/*B* ratio. The results reveal the ultimate tensile strength σ_b of α_2-Ti-25Al-*x*Nb crystals and the elastic moduli (*B*, *E*, *G*) of α_2-Ti-25Al-*x*Nb alloys monotonously increase with the addition of Nb in the whole range of *x*=0-12. Meanwhile a very sensitive ductile/brittle behavior of α_2-Ti-25Al-*x*Nb alloys to Nb content is also detected. The addition of Nb with low content is demonstrated to be profitable for weakening of the brittleness of α_2-Ti_3Al alloys, and the toughening tendency of α_2-Ti-25Al-*x*Nb alloys increases as increasing Nb addition in the range of =0-6. Whereas in the range of *x*=7-9, relative to α_2-Ti_3Al alloys no toughening effect can be seen as Ti in Ti_3Al being partially substituted by Nb. As *x*≥10, the toughening effect of Nb addition is activated again, and an obvious improvement in the ductility and strength of α_2-Ti-25Al-12Nb alloy is observed as comparing with α_2-Ti-25Al-6Nb alloy. For this toughening and strengthening effect of Nb addition a reasonable explain was given by means of the analysis of the density of states (DOS) and the projective density of states (PDOS) of α_2-Ti-25Al-*x*Nb (*x*=0, 6, 7, 12) crystals.

Keywords: α_2-Ti_3Al Nb alloying mechanical property first-principles calculation

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通讯作者: 彭平

作者简介: 曾宪波, 男, 1984年生, 硕士生

作者Email: pppeng@hnu.cn

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