Fermi surface calculations of Cu_3Au

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A study is presented of the calculated Fermi surface of the noble-metal binary alloy Cu_3Au, which has attracted much attention because of the classical order-disorder phase transition found at 663K. Comparisons are made between results obtained for the simple cubic Cu_3Au and the face centered cubic Cu lattices using the standard ab initio crystal structure suite WIEN2k. Results are shown for bulk electronic band structures, densities of states (DOS) for individual atoms and cuts across the Fermi surface.

1. Introduction

This work presents calculations to illuminate the Fermi surface of the noble-metal binary alloy Cu_3Au, which has attracted much attention because of the classical order-disorder phase transition found at 663°K. The bulk electronic band structure has previously been studied by various first principle approaches and there exists some photo-emission experimental results [1]. In particular insight might be obtained by comparing cuts across Fermi surfaces between experimental and calculated Fermi surfaces, as has previously been carried out for magnetic systems [2]. Accordingly, this initial study presents results to be compared with experimental Fermi surface measurements using photo-emission being carried out by the LaTrobe University Group (Prof. R. Leckey and colleagues). In particular recent extensions of the standard ab initio crystal structure suites WIEN2k [3] allow the calculation of Fermi surfaces by use of the XCrysDen package [4]. The present work presents preliminary results from this package as implemented on the VPAC computer cluster.

It is well known that Cu is a text book example of the close packed face centred cubic structure. On the other hand Cu_3Au is simple cubic (sc) structure where the corner atoms of the fcc Cu lattice are replace by gold atoms. Accordingly the Brillouin zones are somewhat different, but still of standard form as shown in Figs. 1 and 2, which also illustrate the nomenclature of the principal symmetry directions used in electronic band structure plotting.

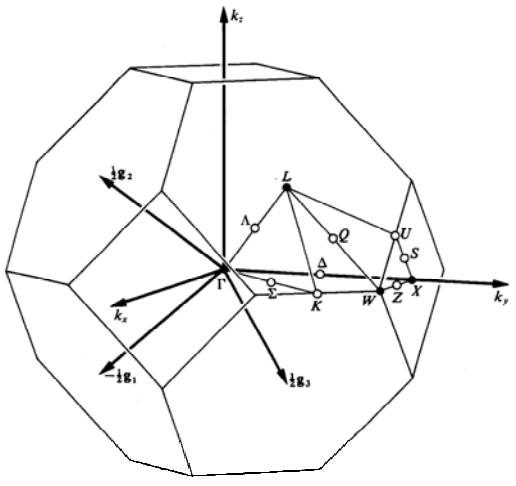

Fig. 1. fcc Brillouin zone with standard notation [5].

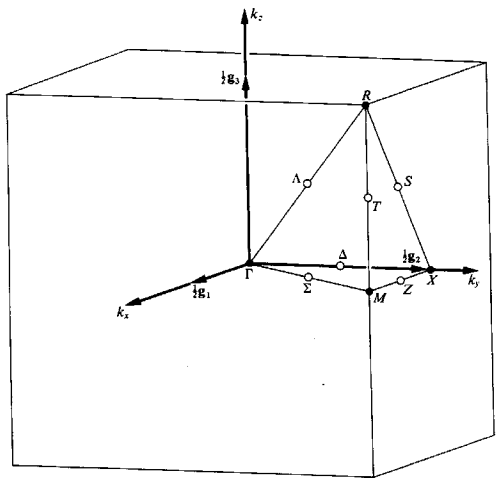

Fig. 2. sc Brillouin zone with standard notation [5].

2. Method of Calculation and Results

Calculations have been performed using the WIEN2k ab initio crystal properties computer suite [3]. The calculations are performed with experimentally determined lattice parameters in the density functional picture, using the generalized gradient approximation (GGA) with the linearised augmented plane wave plus new local orbitals method (LAPW +lo). In particular, they allow the identification of electronic structure with atomic orbitals.

Fig. 3 compares results of electronic band structure calculations for Cu_3Au (left) with Cu (right). The Cu results can be divided into three energy regions, with nearly free electron behaviour at both high and low energies, but with flat bands in the middle range around the Fermi level. On the other hand Cu_3Au shows more features and in particular more than one band intersects the Fermi level.

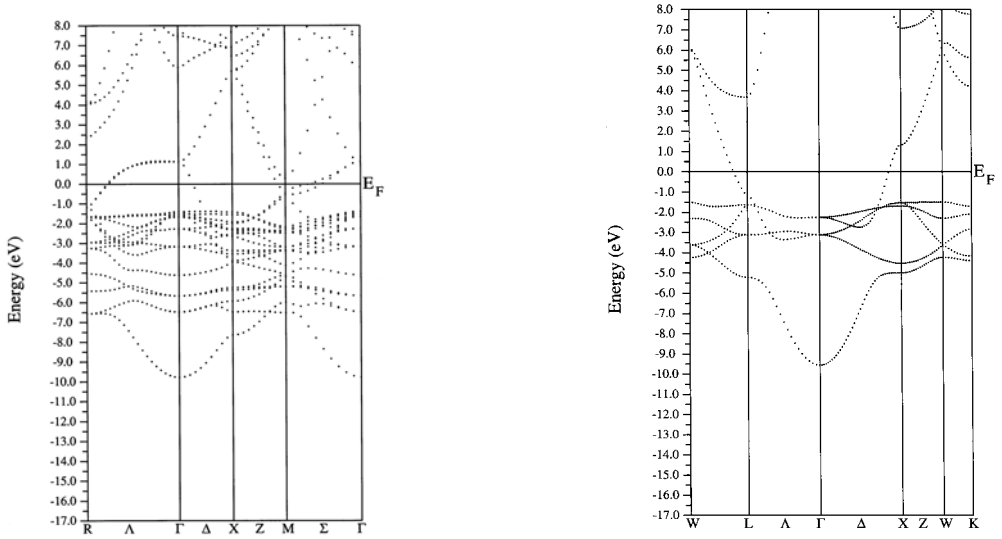

Fig. 3 Comparison of electronic band structure for Cu_3Au (left) with Cu (right). Note that in the case of Cu_3Au more than one band intersects the Fermi level denoted by E_F. The principal symmetry directions are as denoted in Figs. 1 and 2 respectively.

It is possible to assign atomic orbitals to the various bands by considering the contributions from the density of states (DOS) of the contributions from the Cu and Au atoms as shown in Figs. 4 and 5. Inspection of the figures suggest that the upper part of the conduction bands are dominated by the Cu states, whilst the lower part is dominated by the Au states [1]. Compared with earlier work [1] the present calculation extends this interpretation as it covers more of the Brillouin zone.

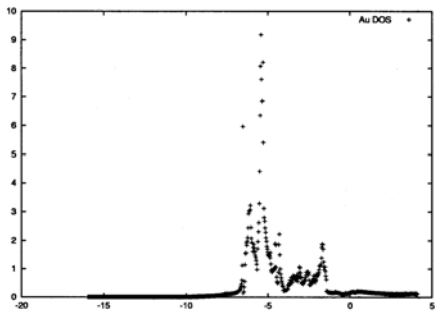

Fig. 4. Contribution of Cu and Au sites in Cu_3Au total DOS versus energy in eV.

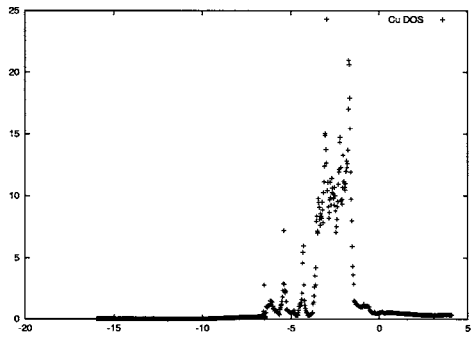

Fig. 5. Contribution of Cu and Au sites in Cu_3Au total DOS versus energy in eV.

Fig. 6 shows the results of considering states close to E_F (=0 eV) for the plane defined by the line Σ and line Λ of Fig. 2 for different energy bands. In the diagrams Γ is the centre of the base plane, the four corners are R points and the centres of the sides of the base plane are given by two X and two M points respectively.

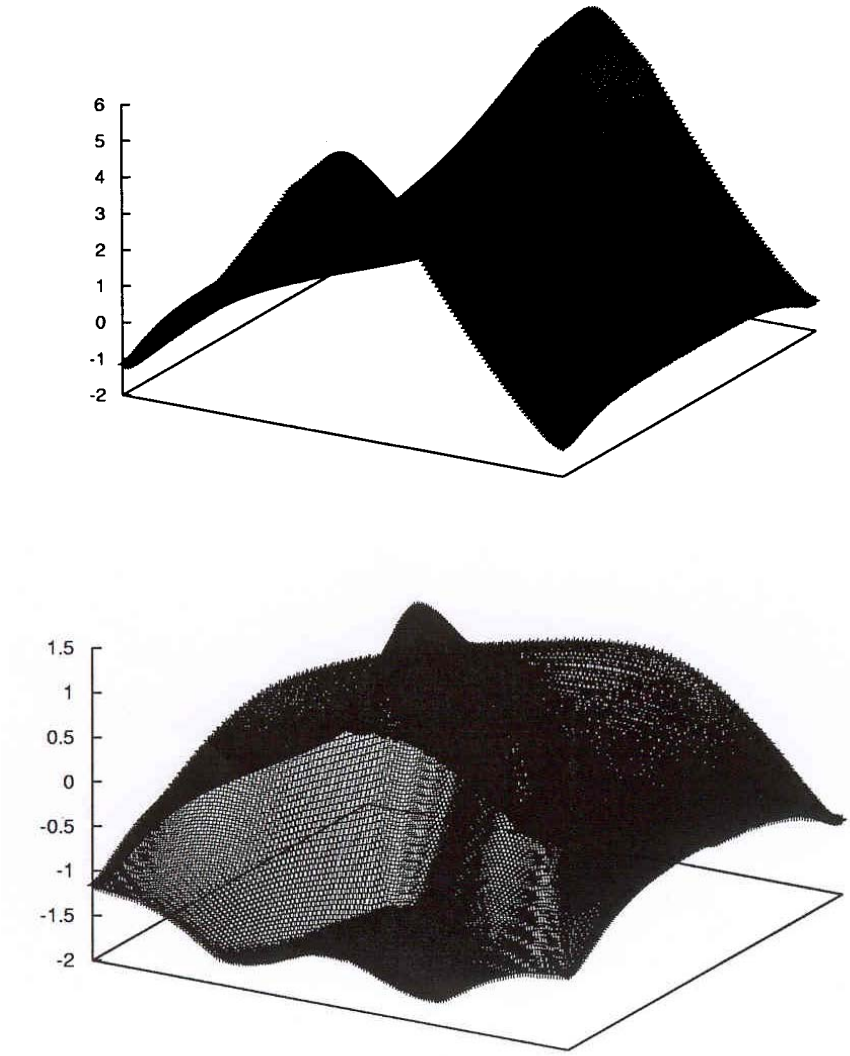

Fig. 6. Energy values in eV close to the Fermi surface (plane through z axis at 0 eV) in the plane containing the lines Σ and lines Λ (compare Fig. 2) for two different energy bands that both cross the Fermi surface.

References

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