# A-8. THREE-DIMENSIONAL CRYSTALLIZING COMBINED π-BONDING ORBITALS("O"S' BONDING\*) AND ELECTRICAL AND MECHANICAL PROPERTIES OF ALLOY METALS

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#### **ABSTRACT**

The "O"S' BONDING make metallic and non-metallic crystal structures and form localized superconducting orbitals, which induce electrical conduction, semi-conduction, and superconduction. The orbitals are proved by Ampere's law, Faraday's law, Meissner effect, high critical temperature of the copper oxide layers, abnormal trans-membrane signal in cancer cell and plastic deformations by twins and dislocations. In the case of alloying metals, the most detrimental cases of electrical conduction are those of solid solution and intermetallic compound. The highest case for the hardness are also those of solid solution and intermetallic compound. It explains the contributions of the "O"S' BONDING for conduction bands and plastic deformation by twins and dislocations.

#### 1. EXPERIMENTAL EVIDENCES

# 1-1. ELECTRICAL CONDUCTION BY LOCALIZED SUPERCONDUCTING OBRITALS AFTER AGING AND CREEPING OF POLYCRYSTALLINE METAL

In recent research the grain crystal in polycrystalline structure rotates during aging, creep and fatigue process by viscous shear strain. The crystalline elastic anisotropy of the grain emerges more and more with the rotation by deforming.

Many aging and creep tests show that electrical resistivity reduces as the creep time elapses. They also show that resistivity temperature coefficient increases as the anisotropy channeling at the grain boundaries increases but temperature independent resistivity decreases surprisingly (Ref.1, Ref.2 and Ref.3)

It means that any localized superconductivity in room temperature increases with the increasing elastic anisotropy's channelings at the grain boundaries (Ref.4). It also suggests that superconduction composes of two steps, in which the first is the localized orbital's superconduction and the second is the trans-orbital superconduction. It is thought that metals begins the localized superconduction at the onset of solidifying crystallization from liquid and

<sup>\* &</sup>quot;O"S' BONDING is a short name of the THREE-DIMENSIONAL CRYSTALLIZING COMBINED  $\pi$ -BONDING ORBITALS, which means that it looks like alphabet "O"s being three dimensionally bonded with regularity.

it has been called normally conduction band. The squares and hexagonal planes in real structures satisfy the Kronig-Penney cyclic potential model of closed ring type which suggests the localized superconducting band. And also the band was discovered experimentally in case of Y Ba<sub>2</sub> Cu<sub>3</sub>  $O_{6.9}$  as in Fig.1 (Ref.5).

# 1-2. NEW METALLIC BONDING ORBITAL, NORMAL CONDUCTION AND SUPERCONDUCTION

Electrical conduction is due mainly to new metallic bonding orbitals, which are localized interatomic superconducting rotational electron pairs orbitals formed by elastic anisotropic channeling (Ref.4) (Ref.6). Normal conduction electrons move from one metallic orbital to next one with the aid of electric potential field as in Fig.2(c). Superconduction electrons move form one orbital to next one without electric potential field by pair with the aid of only coulomb forces in the next orbitals domain because the resonance in the elastic anisotropic channeling needs even number of atoms and even number of electrons and therefore the normal rotating electron pairs orbital consists always of electron pairs as in Fig.2(d).

The highly accelerated rotating orbital transfers electron pairs form one orbital to next one without electric potential field. It is the superconducting state or trans-orbital superconducting state. Face centered cubic structure has square and hexagonal planes of elastic anisotropic channeling in Fig.2(b). Body centered cubic structure has square planes of elastic anisotropic channeling. Closed packed hexagonal structures has hexagonal planes of elastic anisotropic channeling. It is believed generally that the structure that has more the elastic anisotropic channeling planes is more advantageous for better conduction. It seems that these orbitals be called three-dimensional crystallizing combined  $\pi$ -bonding orbitals. The copper oxide layers have high  $T_c$  because they have oxygen atoms between copper atoms in the square elastic anisotropic channeling and the oxygen atoms also attracts rotating electrons to the next orbitals domain as in Fig.3.

#### 1-3. SEMICONDUCTION

Semiconductors have diamond cubic structure, Sphalerite structure and wurtzite structure. If temperature is raised, the electrons in the covalent bondings are promoted to the new metallic bonding orbitals of the elastic anisotropic channeling by thermal energy vibration. The elastic anisotropic channels in diamond cubic and sphalerite structures are FCC base atoms and also HCP lower and upper base atoms in wurtzite structure. The base atoms of elastic anisotropic channeling make the new metallic bonding orbitals with the promoted electrons by the thermal phonon and make the conduction bands or the localized interatomic superconducting orbital (Ref.6).

#### 1-4. AMPERE'S LAW

The discovery that currents produce magnetic effects was made by Oersted in 1820. This leads to the "right hand rule" for finding the direction of B near a wire carrying a current I. The right hand rule can be easily explained by the localized interatomic superconducting rotational

electron pairs orbital formed by elastic anisotropic channeling (or new metallic bonding orbital).

Fig.4 shows that transverse and cross-sectional arrays of the localized superconducting orbitals make the magnetic field of right hand rule. The centrifugal coulomb forces and the rotational electrons on the orbitals in the transverse array make the magentic field. But the cross-sectional arrays dont's make it because the rotational electrons in the both directions have same numbers and velocities (Ref.7).

The law of Biot and Savart is used for practical problems in replace of Ampere's law. The basic principles are same for both laws.

#### 1-5. FARADAY'S LAW

Faraday had the insight to perceive that the change in the flux  $\Phi_{\rm B}$  for the left coil in Fig.5 is the important common factor of magnetic induction. This flux may be set up by a far magnet or a current loop. Faraday's law of induction says that the induced emf  $\mathcal E$  in a circuit is equal to the negative rate at which the flux through the circuit is changing.

Fig.6 shows that trans-orbital moving of electrons is induced by any change of magnetic flux. Because both clockwise and counter-clockwise rotating electrons in the orbital have same numbers, the resultant magnetic flux is zero. But if any magnetic flux is loaded in the loop of the coil the magnetic flux outside the wire will be unbalanced and this produces induced current. The induced current reproduces an induced magnetic flux. Finally the external magnetic field becomes zero (Ref.7). It also automatically satisfies the Lenz's law that the induced current appears in such a direction that it opposes the change of the flux that produced it.

#### 1-6 MEISSNER EFFECT

In the case of trans-orbital superconducting state, the induced electrons circulate near the surface. The electrons inside the material come out near the surface through the three dimensionally connected localized superconducting orbital. The circulating electrons make the induced magnetic field by Ampere's law. Finally the magnetic flux becomes zero inside the material and becomes more stronger outside the material. This is the Meissner effect. The stronger flux outside the material maintains the induced current near the surface. If the induced current exceeds the limit for the superconducting trans-orbital coulomb's force between the localized orbitals, the material returns to normal conduction state. And also if there are any regions which are not connected through the three-dimensionally interconnected localized orbitals, they becomes fluxoids, which increase critical magnetic flux and critical current because they offer greater area for the currents circulating with the superconducting trans-orbital coulomb's force (Ref.7).

### 1-7. ABNORMAL TRANS-MEMBERANE SIGNAL IN CANCER CELL

An understanding of the mechanisms responsible for the control of normal proliferation and differentiation of the various cell types which make up the human body will undoubtedly allow a greater insight into the abnormal growth of cells. Particular attention is now focused on the role of polypeptide growth factors as molecular which may play a central role as both positive and negative regulators of normal and abnormal growth control and development. A large body of biochemical evidence was eventually used to generate a receptor model with an external ligand binding domain linked through a single trans-membrane domain to the cytoplasmic tyrosine kinase and autophosphorylation domains (Fig. 7).

The ligands induced conformational change in the external domain generates either a push-pull or rotational signal which is transduced from the outside to the inside of cell. The ligand gives electron pairs to the receptor, The electron pairs are energy-leveled at  $\sigma$ -bonding orbitals by ligand field theory. Abnormal signal without ligand reaction in cancer cell is from the microstructure of the crystalline receptor material (abnormal proteins) (Ref.8), which is elastically anisotropically channeled by the lesions of its related DNA (its stressing, oncogenic virus and various kinds of carcinogens). The  $\alpha$ -helical polypeptide structures of the receptors (Fig.8) can be packed by nitrogen atoms, which have remaining valence electrons and make three-dimensional crystallizing combined  $\pi$ -bonding orbitals (Fig.2(a) and (b)). They may be square, hexagonal and combinations of square and hexagonal. They are such as FCC, BCC and HCP of metallic crystal structures. Polypeptidic  $\alpha$ -helical amino-acids in liquid state can be packed in solid-crystallized state by the three -dimensional crystallizing combined  $\pi$ -bonding orbitals in such a way that the liquid metal be solidified by the crystallization.

If the nitrogen atoms are packed by the crystallization they pull any kinase without the ligand-induced conformational change by the crystallization attraction force.

It is thought that the normal ligand-induced conformational change makes an elastic anisotropic channeling of square, which pull the kinase (normal signal).

# 1-8. DISTRIBUTION OF NOES IN THE PROTO-ONCOGENIC AND ONCOGENIC FORMS OF THE NEU PROTEIN

The three dimensional structure of the trans-membrane region of the proto-oncogenic and oncogenic forms of the neu protein is shown in Fig.9 (Ref.9).

The NMR results Fig. 10 show that the proto-oncogenic and oncogenic structures are both  $\alpha$ -helical and are within experimental limits, essentially identical. There is no evidence for any gross distortion of the helices dependent upon the type of amino acid side chain of residue 12. These results therefore do not support the model involving local conformational difference between the mutant and wild-type receptors. In the NMR work reported here however, no direct evidence was found in support of dimerization of either peptide. Evidence for dimers might have been detected through anomalous NOEs and the observation of differences following ionization of the glutamate side chains since this would be expected to disrupt the putative inter-molecular hydrogen bonds between them (Ref. 10).

The model building shows that the structures determined by NMR are quite capable of forming the proposed  $\alpha$ -helical packing. The increased numbers of NOEs in amide residues are caused

by three-dimensional crystallizing combined  $\pi$ -bonding orbitals of the packed nitrogen atoms. The polypeptidic  $\alpha$ -helical amino-acids in liquid state can be packed in solid-crystallized state by the three-dimensional crystallizing combined  $\pi$ -bonding orbitals in such a way that the liquid metal be solidified by the crystallization.

If the nitrogen atoms are packed by the crystallization they pull any kinase without the ligand-induced conformational change by the crystallization bonding force.

The increased numbers of NOEs in side chain residues in Fig. 10 might be caused by a packing of the atoms, in which the atoms have remaining valence electrons and make the three-dimensional crystallizing combined  $\pi$ -bonding orbitals.

#### 1-9. PLASTIC DEFORMATIONS BY TWINS

Fig. 11 shows two models for plastic deformation. Fig. 11(a) is one model for slip deformation and Fig. 11(c) is the other model for twin deformation. Fig. 12 is the stress-strain curve when twins occur. Fig. 13 shows twin plane and twin direction for each crystal model. The orientations of lattice are not variant for the dislocations during deformation while they are variant for twins. The moving distance is one atom's diameter for the dislocations while it is much less than one atom's diameter for the twin. The twinning is a reorienting of a crystal system on the easiest planes and directions. Twinning is an atom's moving and an reorienting from one  $\pi$ -bonding orbital to other oriental  $\pi$ -bonding one in the three-dimensional crystallizing combined  $\pi$ -bonding orbitals. Twinning makes a micro-plastic deformation under low fluctuating fatigue stress and under constant low stress in creep state. The micro-plastic deformation by twinning occurs in the crystal grains of polycrystalline materials. The different rotational micro-plastic deformations of the grains make many micro-cracks at the grain boundaries, which propagate, grow and reach to final failures of the fatigue and creep.

#### 1-10. PLASTIC DEFORMATIONS BY DISLOCATIONS

Fig.14 shows the lattice structure of edge dislocation. Fig.15 shows the process of the plastic deformation by edge dislocation. Fig.16 shows lattice structure of screw dislocation. The burg's vector is perpendicular to the slip plane in the case of edge dislocation while it is parallel to slip plane in the screw dislocation. The plastic deformation by edge and screw dislocations is an atom's moving from one  $\pi$ -bonding orbital to the next same oriental  $\pi$ -bonding one in the three-dimensional crystallizing combined  $\pi$ -bonding obitals ("O"S' BONDING). An atom in "O"S' BONDING attends on many  $\pi$ -bonding orbitals. Even if an atom is picked out from the packing, the packing can not be destroyed. If the atom returns to the picked out point, it will be packed again by restoring the destroyed  $\pi$ -bonding orbital. This means that new atoms can be packed continuously by making new  $\pi$ -bonding orbitals and can be crystallized very systematically. It is from the above fact that the packed abnormal receptors composed by amino acids pull any kinase without any conformational change by external ligands' reactions.

## 1-11. HARDENING MECHANISMS

Fig.17 shows crystal grain boundaries. The grain boundaries make it difficult for dislocation moving because the next same oriental  $\pi$ -bonding orbitals can not be connected easily at the grain boundaries. As the grain size is smaller the strength is higher therefore. Fig.18 shows motion of a dislocation through a row of obstacles by the Orowan process. The obstacles also make it difficult for dislocation moving because the next same oriental  $\pi$ -bonding orbitals can not be easily connected at the obstacles.

## 2. ELECTRICAL AND MECHANICAL PROPERTIES OF ALLOY METALS

## 2-1. ELECTRICAL PROPERTIES OF ALLOY METALS

Fig.19 shows the relationships between electrical conductivity and concentration of alloying metals in cases of eutectic, continuous solid solution, partially miscible solid solution and intermetallic compound. The most detrimental cases for electrical conduction are those of solid solution and intermetallic compound. It explains the contributions of the "O"S' BONDING as the localized superconducting orbitals or the conducting bands. The solid solution has size difference while the intermetallic compound has ionic or covalent bonding. The eutectic structure is less detrimental to electrical conduction because the localized superconducting orbitals ("O"S' BONDING) meet at the boundaries of the mixed crystals.

## 2-2. MECHANICAL PROPERTIES OF ALLOY METALS

Fig.20 shows the relationships between mechanical hardness and concentration of alloying metals in the same case as Fig.19. The highest cases for the hardness are also those of solid solution and intermetallic compound. It explains the contributions of the "O"S' BONDING for plastic deformations by twins and dislocations. The size difference of the atoms in the solid solution and the ionic or covalent bonding of the intermetallic compound disturbs the formation of the "O"S' BONDING. Fig.21 shows various mechanical properties in cases of intermetallic compound and peritectic alloying metals. The ultimate tensile strength, yield strength and elongation percentage have some relationships with the hardness.

# 2-3. EVIDENCES FOR ELECTRICAL CONDUCTION BY LOCALIZED SUPERCONDUCTING ORBITALS("O"S" BONDING)

Fig.22 shows mechanical and electrical properties for Ni-Cu alloys(Ref.13). The resistivity temperature coefficient increases as the alloys become purer state. It means that thermal vibrations of the atoms hinder the electrical conduction more seriously in case of pure state. It implies that the pure state has stronger localized superconducting orbitals and also the electric conduction occurs by the localized superconducting orbitals. It is in good agreement with the results of(Ref.14) that the formation of stronger localized superconducting orbitals at the grain boundaries by rotating crystal grains increases electrical conductivity and resistivity temperature coefficient. It is also experimentally evidenced that conductive polymers have

connective localized superconducting  $\pi$ -bonding orbitals such as polyacetylene, polyaniline, polypyrrole, polythiophene, polyfuran and polyindol (Ref.14).

#### 3. CONCLUSIONS

1. The most detrimental cases for electrical conduction are those of solid solution and intermetallic compound. It explains the contributions of "O"S' BONDING as the localized superconducting orbitals or conducting bonds.

2. The highest cases for the hardness are also those of solid solution and intermetallic compound. It explains the contributions of the "O"S' BONDING for plastic deformations

by twins and dislocations.

3. Electrical resistivity temperature coefficient and electrical conductivity increase as the alloys become purer. It suggests the electrical conduction by the localized superconducting orbitals.

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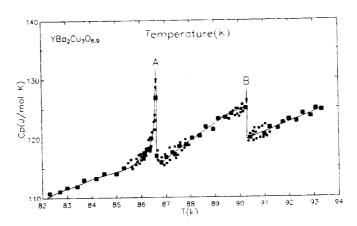


Fig. 1. Heat capacity of Yba $_2$  Cu $_3$  O $_{6.9}$  vs. temperature

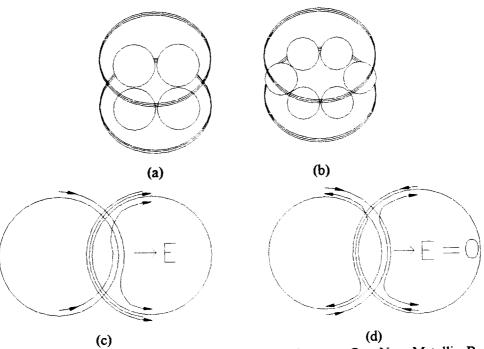


Fig.2. Mechanism of Conduction and Superconduction between One New Metallic Bonding Orbital and the Next

- (a) square unit set of new metallic bond
- (b) hexagonal unit of new metallic bond
- (c) conduction
- (d) superconduction

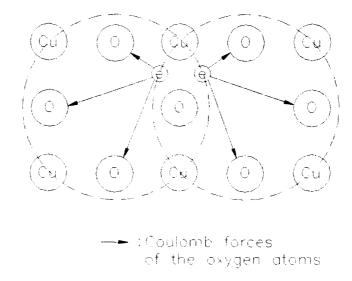


Fig.3. Copper oxide superconductor

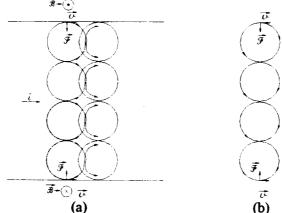




Fig.4. Cause of magnetic field B by coulomb forces and moving charges in the conducting wire.

- (a) transverse array of the localized interatomic superconducting orbitals along the wire.
- (b) cross-sectional array of them.

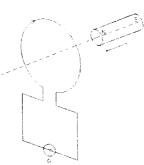


Fig. 5. Galvanometer G deflects which the magnets is moving while the magnet is moving with respect to the coil

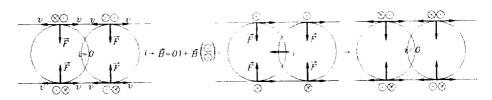


Fig.6. Trans-orbital moving of electrons induced by any change of magnetic flux (Faraday's law of induction)

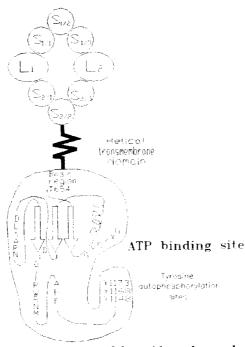


Fig.7. A model for the structure of the epidermal growth factor

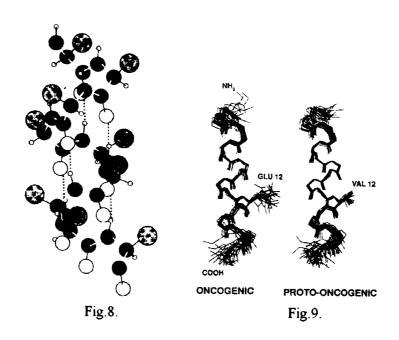


Fig. 8.  $\alpha$  -helical polypeptide structures Fig. 9. Twenty-two oncogenic and 22 proto-oncogenic

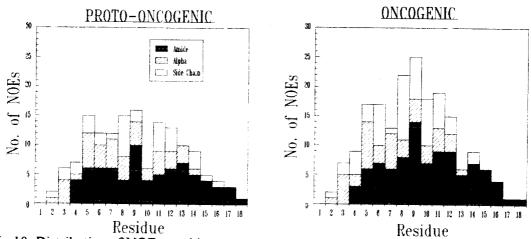


Fig.10. Distribution of NOEs used in structure calculations. Each atom involved in an NOE is indicated: for example an  $\alpha$  H-NH restraint is recorded for both the  $\alpha$  and the amide proton.

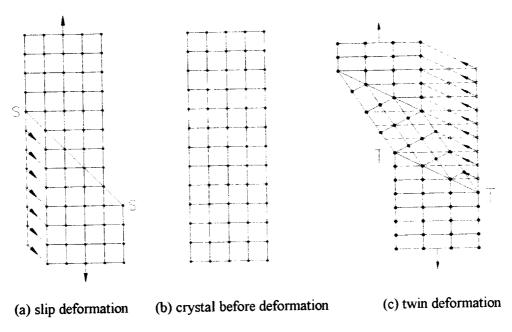


Fig.11 model for plastic deformation

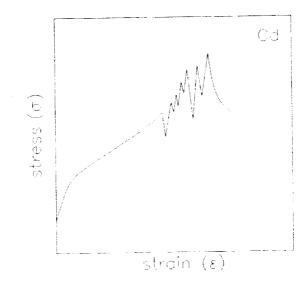


Fig.12 stress-strain curve at twin formation

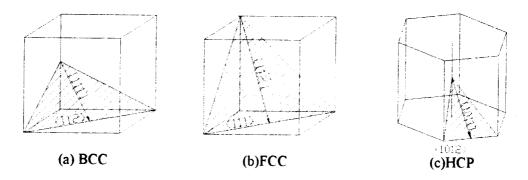


Fig.13 planes and directions for twins

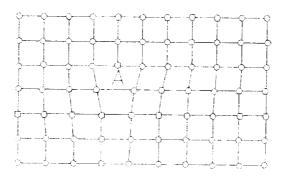


Fig.14 The center of edge dislocation

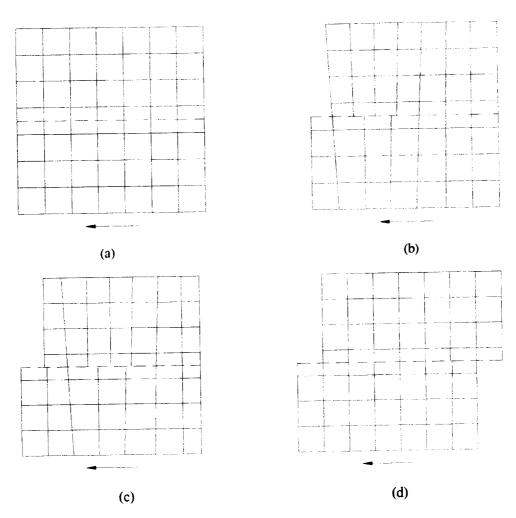


Fig.15 The process of the plastic deformation by edge dislocation

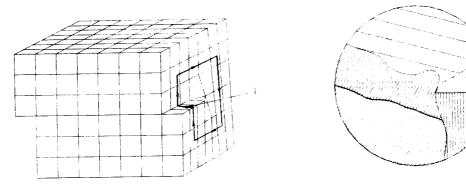


Fig.16 Screw dislocation

Fig.17 crystal grain boundaries

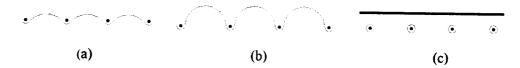


Fig.18 Motion of a dislocation through a row of obstacles by the Orowan process

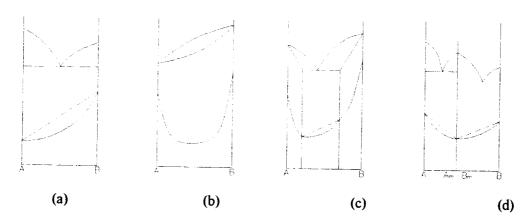


Fig.19 Relationships between electrical conductivity and concentration of alloying metals

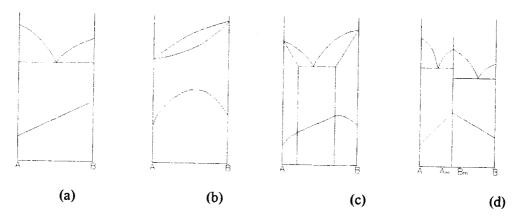


Fig.20 Relationships between mechanical hardness and concentration of alloying metals

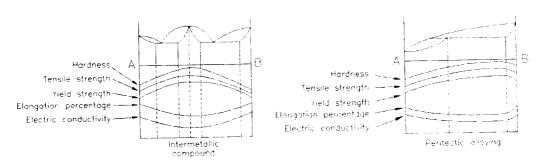


Fig.21 Mechanical properties pf intermetallic compound and peritectic alloying metals

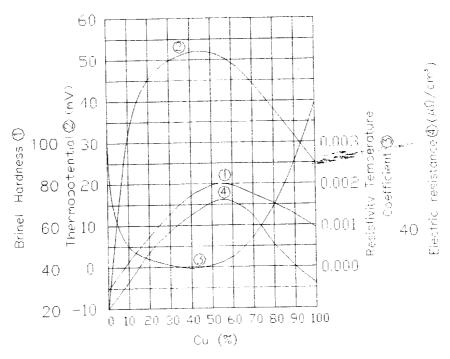


Fig.22 Mechanical and electrical properties for Ni-Cu continuous solid solution alloys