bcc α-ferrite (α-Fe) [2], α'-martensite (α'-Fe) and fcc γ-austenite (γ-Fe) [2]. α-Fe and γ-Fe form under thermo-dynamically stable condition while α'-Fe and ε-Fe are kinetically stable phase. However, ε-martensite (ε-Fe) has hexagonal crystal structure with parameters of a=2.45 Å and c=3.93 Å. Formation of needle-like ε-Fe (Fig.1a) was found to have contributed to the high strength of non-magnetic Mn-containing austenitic stainless steel . Electron diffraction in Fig.1b reveals the composite pattern from zone axes of $<0001>_\varepsilon$//$<111>_\alpha$. The formation of・ε-Fe in this case is due to Mn concentration and hence, lowers SFE.The formation of Zigzag chips was attributed to the formation of ε-Fe during high speed cutting of 304 and 316, as shown in Fig.2.

1. T. Takajashi and W. A. Bassett, Science, 1964, 145, 483-484.
2. P. Villars and L. D. Calvert, Pearson's Handbook of Crystallographic Data for Intermetallic Phases, Vol3, ASM, Metals Park, 1985, 2162.
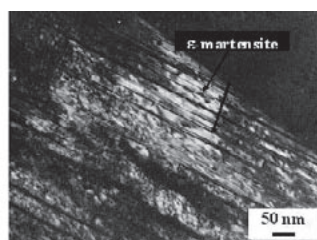3. H. Holmberg, J.-O. Nilsson and P. Liu, ISIJ Intern. 1990, 30, 594-599.

Fig.1a. Formation of needle-like ε-Fe in a non-magnetic Mn-containing austenitic stainless steel
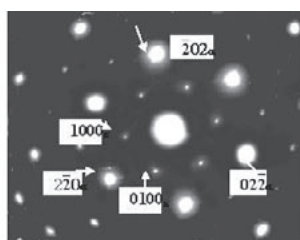
Fig.1b. Composite electron diffraction from the $<0001>_\varepsilon$//$<111>_\gamma$.
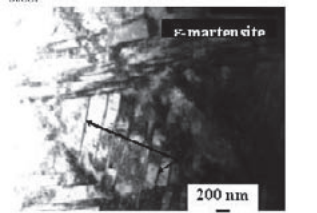
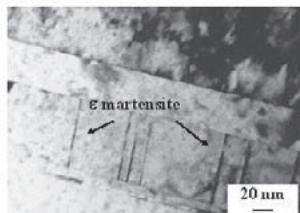Fig 2a. Formation of ε-Fe in 304 stainless steel during high steed cutting.

Fig 2b. Formation of ε-Fe in 316 stainless steel during high steed cutting.

Keywords: martensites, stainless steels, TEM

P08.14.140

Structure of homologous series $Zn_k(In,Ga)_2O_{k+3}$ of as thermoelectric materials

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Homologous compounds $Zn_kIn_2O_{k+3}$ are ones of candidates for good thermoelectric and transparent conducting materials and the performances are being improved by partial substitution of Zn or In, and so on. The homologous compounds are reported to be stable when k in $Zn_kIn_2O_{k+3}$ is 3 or over, and the electrical conductivity increases as k decreases, as a result of increased carrier concentration. The trend in electrical conductivity tells that the lower k member would show the higher electrical conductivity when the member could be prepared. According to our previous work, substitution of In by Ga stabilized the structure of homologous compounds even for k=1 and 2. In this presentation, the results of crystal structural analysis for $Zn_k(In,Ga)_2O_{k+3}$ (k=1, 3, 5) by X-ray Rietveld analysis are shown and the relationships between the structure and the physical properties are discussed. The basic structure of the compounds consists of InO_2^- and $(In,Ga)Zn_kO_{k+1}^+$ layers alternately stacked along the c-axis to have a space group of R-3m. Edge-shared InO_6 octahedra form the continuous InO_2^- layer on the c-plane. The results of structural analysis indicated that the longer In-O length in the InO_2^- layer is attributable to the higher electrical conductivity. Band structure of $Zn_3In_2O_6$ are also evaluated by first-principle calculation (CASTEP), using the structural data obtained from the Rietveld analysis. Considering the electronic structure and the formation enthalpy, $Zn_3In_2O_6(4)$ in which In^{3+} in the $InZn_3O_4^+$ layer occupies the tetrahedral site preferentially, is likely to be the favored structure.

Keywords: Rietveld analysis, relation between structure and thermoelectricity, band calculation

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X-ray crystallography and NMR spectroscopy in unrevealing the catalytic mechanism of a peroxiredoxin

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The protozoan parasite Trypanosoma cruzi is the causative agent of Chagas' disease. In Latin America, 16-18 million people are infected by the parasite creating a major health problem. The disease is fatal in 15-30% of those infected while others are inflicted by serious disabilities. Drugs currently used in the treatment of Chagas' disease often have toxic side effects and fail to clear parasitaemia and their mode of action is unknown. One of these drugs, nifurtimox, undergoes redox cycling with the parasite. Reactive oxygen species (ROS), such as hydroperoxides, are the unwanted by-products of aerobic metabolism. To protect cells against their potentially lethal effects a series of pathways have evolved that are collectively called the oxidative defence system. Uniquely, trypanosmatidae contain several enzyme-mediated pathways for the removal of hydroperoxides that are centred upon the unusual thiol trypanothione and are potential therapeutic targets. We have investigated one of the key terminal peroxiredoxins from this system, glutathione peroxidase I (TcGPXI). By using X-ray crystallography, NMR spectroscopy, site-directed mutagenesis and enzymatic assays we were able to unravel the catalytic mechanism of this enzyme. Crucially, we have shown that despite significant sequence homology to the glutathione-dependent peroxidases the catalysis, in contrast, involves atypical 2-Cys peroxiredoxin mechanism. The mechanism relies on a significant conformational change including unravelling of an alpha helices and formation of a disulphide bridge. We have identified the role of the specific Cys residues in the structure and investigated TcGPX in oxidized and the fully reduced form in the presence and absence of a substrate.

Keywords: catalytic mechanisms, dynamic properties, conformational change

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