

P-512

DIFFRACTION PLANE DEPENDENCY OF ELASTIC CONSTANTS
IN FERRITIC STEEL IN NEUTRON STRESS MEASUREMENT

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ABSTRACT

Neutron diffraction measurements have been made to investigate the elastic properties of the ferritic steel obtained from socket weld. The Kroner elastic model is found to account for the $[hkl]$ -dependence of Young's modulus and Poisson's ratio in the material. Maps of residual stress are later to be made by measuring lattice strain from shifts in the (112) diffraction peak, for which the diffraction elastic constants are herein found to be $E=243 \pm 5 \text{ GPa}$ and $\nu=0.28 \pm 0.01$.

INTRODUCTION

Neutron diffraction is the only method available to determine non-destructively the residual stresses inside weldments. Thermal neutron are generated inside a nuclear reactor, and are emitted through beam tubes to be diffracted from a squeezed, single-crystal monochromator. The diffracted neutrons have a characteristic wavelength, λ , typically between 0.13nm and 0.26nm. They are shaped into a rectangular beam by masks made of neutron absorbing cadmium. The cross sectional area of the beam is chosen to match the desired spatial resolution in a specimen. Neutrons are scattered from the incident beam direction through angles, 2θ , according to Bragg's law,

$$\lambda = 2d(hkl) \sin(\theta), \quad (1)$$

where $d(hkl)$ is the spacing between atomic planes with Miller indices (hkl)

With a neutron diffractometer, the intensity of diffracted neutrons is measured as function of scattering angle. By fitting the raw neutron data with a gaussian function plus a sloping background, the mean scattering angle of each diffraction peak can be determined to a typical precision of $\pm 0.003^\circ$. The neutron wavelength can also be determined to a high precision, $\pm 1 \times 10^{-5} \text{ nm}$, by calibration against a standard silicon powder specimen, obtained from the National Institute of Standards and Technology (NIST). Hence, values of d_{hkl} can be determined to a precision better than 1 part in 10^4 . Comparing the value of $d(hkl)$ at a location in a weldment with the value, $d_0(hkl)$, in a stress-free sample, provides a

direct measurement of strain, ϵ (hkl), in the atomic lattice,

$$\epsilon$$
 (hkl) = (d(hkl)/d₀(hkl)-1). (2)

The strain is determined in the specimen direction that is parallel to the bisector of the incident and diffracted neutron beams. The principal components of strain are therefore obtained by choosing appropriate specimen orientations.

Assuming that the radial (R), axial (A) and hoop (H) directions are the principal axes of the stress field in a welded tube, and that the material can be treated as a homogeneous elastic continuum, the principal components of residual stress, σ_a , can be calculated directly from the algebraic expression,

$$\sigma_H = \frac{E}{(1+\nu)} \left[\epsilon_H + \frac{\nu}{(1-2\nu)} [\epsilon_H + \epsilon_R + \epsilon_A] \right] \quad (3)$$

where E is Young's modulus, ν is Poisson's ratio and the radial, axial and hoop components of stress, σ_R , σ_A and σ_H , respectively, are obtained by cyclic permutation of the indices in Eq. (3).

When diffraction provides the original data on lattice strains, the elastic constants, E and ν , which appear in Eq. (3) must account for a dependence of elastic properties with direction, [hkl], in a single crystal. A given stress applied in the elastically-soft [200] direction of a single crystal of iron would produce a much larger strain than if it was applied in the elastically-stiff [222] direction. Crystallites embedded in a matrix of polycrystalline material also exhibit an [hkl]-dependence in their elastic response to an applied load. Therefore, to calculate stress from diffraction-measured strains, [hkl]-dependent diffraction elastic constants must be determined. Diffraction elastic constants can be calculated from single-crystal elastic constants[1] by a program[2] based on the Kroner model of elasticity in a polycrystalline aggregate[3]. However, it is preferable to determine the diffraction elastic constants experimentally. This is achieved by applying known stresses to specimens of the material in question and then measuring lattice strain by neutron diffraction from the same (hkl) planes with which the residual stress measurements will be made.

EXPERIMENT

A loading rig was custom-built to fit onto the L3 neutron diffractometer, located at the NRU reactor at the Chalk River Laboratories of AECL Research, Canada. An interface was developed at Chalk River to permit loads to be set automatically, controlled to within ± 0.01 kN and recorded by the neutron diffractometer's data acquisition system. The rig had a maximum load of 50kN and could be operated with the load applied vertically (perpendicular to the scattering vector, for determining Poisson's ratio), or horizontally (parallel to the scattering vector, for determining Young's modulus). The load was set by a screw-driven cross-head, and read by a load cell with a calibration table that was traceable to the National Institute of Standards and Technology (NIST).

A specimen was machined from the base material of a socket weld pipe. The specimen had a cross-sectional area of 21.9 mm², and a gauge length of 50mm. Strain gauges were affixed to the surface of the gauge length to determine bulk-averaged values of Young's modulus and Poisson's ratio for

the material. Readings were taken at irregular intervals during the course of neutron diffraction measurements of lattice strain.

The L3 neutron diffractometer was configured to produce a neutron beam of wavelength 0.10984nm by diffraction from the (117) planes of a squeezed single crystal germanium monochromator. Soller-slit collimators in the incident and diffracted beams restricted the total angular divergence in the scattering plane to be 0.45° and the total vertical angular divergence to be about 3°. The spatial widths of the neutron beams were restricted by masks to be approximately 25mm. After a given load was set on the specimen, a single ³He-based neutron detector was scanned through the (110), (200), (112), (220) and (222) diffraction peaks in steps of 0.1°. Each set of five diffraction peaks was acquired in about 3 hours. Strains were determined through Eqs. (1) and (2), taking as stress-free references, $d_0(110)$, $d_0(200)$, $d_0(112)$, $d_0(220)$, and $d_0(222)$, the lattice spacings measured at zero load. Each lattice spacing was related to the lattice constant, a , through the geometrical relationship $d_{hkl} = a/\sqrt{h^2+k^2+l^2}$. An average value of the stress-free lattice constant, $a = 0.28664 \pm 0.00001$ nm, was obtained from measurements of the five lattice spacings at zero load both in the series of measurements for Young's modulus and in the series of measurements for Poisson's ratio. The typical error in determining strain was $\pm 0.8 \times 10^{-4}$.

RESULTS AND ANALYSIS

The strain gauge readings are plotted in Fig.1, where it is clear that both the Young's modulus and Poisson's ratio data are well-represented by straight lines that have been fit by least square method. The resulting bulk elastic constants are $E = 222 \pm 10$ GPa and $\nu = 0.28 \pm 0.02$.

It is customary in neutron-diffraction strain analysis to choose (hkl) peaks whose elastic properties are similar to those of the bulk material, as measured by strain gauges. These peaks include the (110), (112) and (220), all of whom are expected to exhibit equivalent elastic behaviour. A comparison is made of strains determined by neutron diffraction from the (110), (112) and (220) peaks in Fig.2. All of the data sets are well-represented by a single straight line with slope 243 ± 5 GPa, nearly the same value as obtained by the strain gauges. This line is denoted as the (hhl) line and the strains obtained by averaging (110), (112) and (220) data are denoted as (hhl) strains. A comparison of (hhl) strains and the least-squares lines that fit the strain gauge data is shown in Fig.3 to emphasize that the bulk strains determined by strain gauges are indeed nearly equivalent to strains measured by neutron diffraction from the (110), (112) or (220) peaks. Therefore, as is normally assumed, it is reasonable to apply bulk elastic constants to convert (hhl) strains to stresses through Eq. (3). However, measurements have now been made of the true diffraction elastic constants for (hhl) peaks, $E = 243 \pm 5$ GPa and $\nu = 0.28 \pm 0.01$. These measured values can be used in a future study of residual stresses in socket-welds.

Three data sets, representing strains measured in the stiffest [222], softest [200] and average [hhl] crystallographic directions, are plotted together in Fig.4. Lines are fitted by the least square method to obtain values of Young's modulus that depend clearly on [hkl]. The dependence of Young's modulus on [hkl] is explained very well by the Kroner elastic model calculation[2,3], as presented in Table I. The calculation begins with the single crystal elastic constants for pure iron[1], $C_{11} = 230$ GPa,

$C_{1,2} = 135\text{GPa}$ and $C_{4,4} = 117\text{GPa}$. Young's modulus and Poisson's ratio are calculated for each (hkl) assuming that grains are spherical and the texture is random. The bulk values of Young's modulus and Poisson's ratio for pure iron are 211GPa and 0.29, respectively[1]. These are slightly less than the bulk values determined by strain gauges in the socket weld material. Therefore the [hkl]-dependent Young's moduli that were calculated for pure iron have been scaled by the ratio of the bulk values of Young's modulus to give a prediction of the diffraction elastic constants in the socket weld pipe material. The predicted diffraction elastic constants and the [hkl]-dependent elastic constants determined by neutron diffraction always agree to within twice their standard errors. The Kroner elastic model is therefore confirmed as a valid method to obtain diffraction elastic constants in fine-grained, weakly-textured ferritic steel.

CONCLUSIONS

Strains determined from shifts in the angular positions of the (112) neutron diffraction peak are an excellent approximation to the strains that are measured by strain gauges on bulk material with the same applied stress. Residual stresses can be calculated from (112)-strains through Eq. (3) with the measured diffraction elastic constants, $E = 243 \pm 5\text{GPa}$ and $\nu = 0.28 \pm 0.01$. Even if measurements were not available, the diffraction elastic constants that are calculated by the Kroner method from a combination of single-crystal and bulk elastic constants in the literature are reliable for socket-weld ferritic steel.

REFERENCES

- [1] Smithells Metals Reference Book, 6th edition, Eric A. Brandes ed., Butterworth and Co. (Publishers) Ltd., 1983.
- [2] H. Behnken and V. Hauk, Z. Metallkde. 77 (1986), 620-625.
- [3] E. Kroner, Z. Physik 151 (1958) 504-518.

Table I. Comparison of the hkl-dependent elastic constants.

BULK ELASTIC CONSTANTS			
	Pure Iron	Socket Weld Pipe Material (by strain Gauges)	
Young's Modulus (GPa)	211	222	
Poisson's Ratio	0.29	0.29	
DIFFRACTION ELASTIC CONSTANTS			
	(hkl)		
	(200)	$\langle hhl \rangle$	(222)
<u>Calculated for Pure Iron</u>			
Young's Modulus (GPa)	174	224	248
Poisson's Ratio	0.33	0.28	0.25
<u>Scaled by Bulk Values</u>			
Young's Modulus (GPa)	183	236	261
<u>Neutron Diffraction</u>			
Young's Modulus (GPa)	182	243	268
Poisson's Ratio	0.31	0.28	0.30

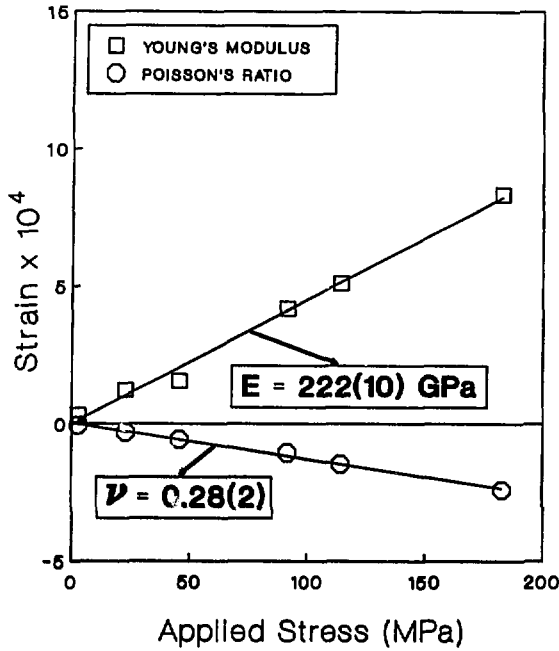


Fig.1 Measurements of Young's modulus and Poisson's ratio by strain gauges.

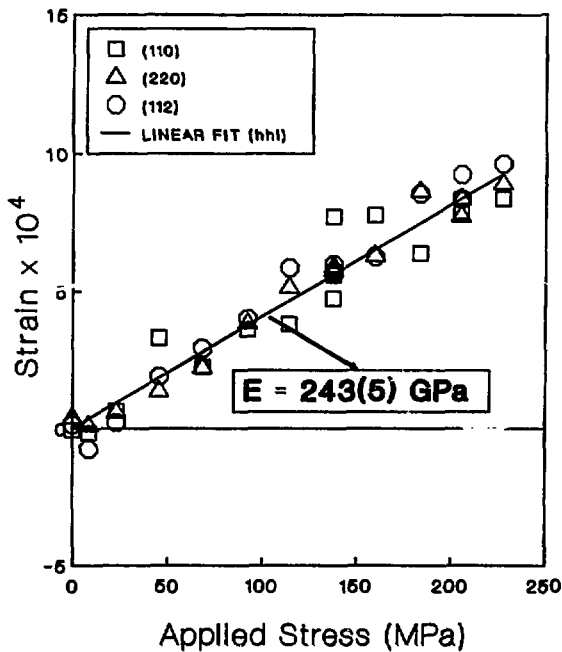


Fig.2 Strains determined by neutron diffraction for (110), (112) and (220) planes.

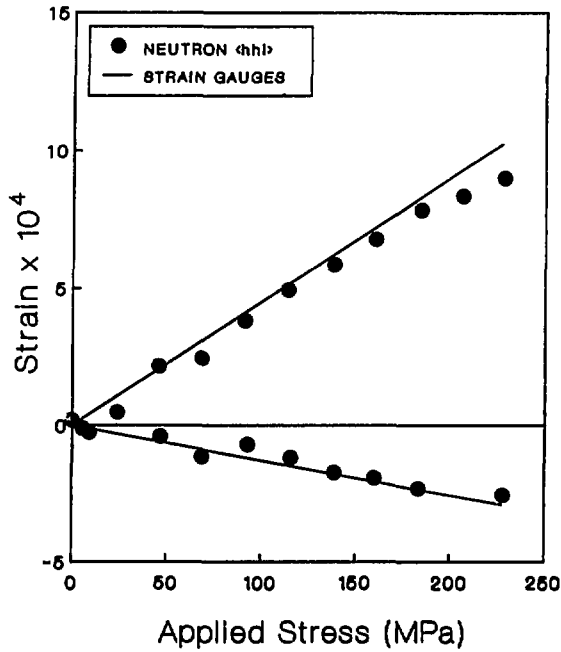


Fig.3 Comparison of averaged (hhl) strains obtained by neutron diffraction and least square fit of strain gauge data.

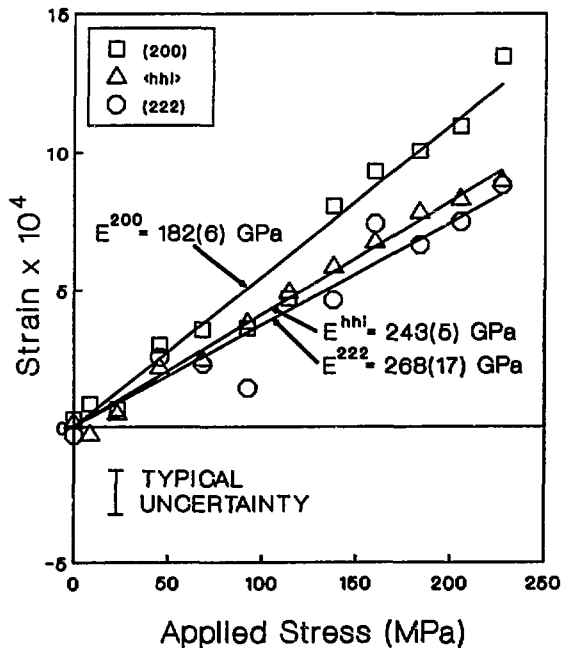


Fig.4 Strains determined by neutron diffraction for elastically soft (200) and stiffest (222) planes.