

# Analytical Simulation of Hydrogen Induced Internal Loading on Metals

張國益、王啟聖 ; 劉大銘

E-mail: 9707293@mail.dyu.edu.tw

## ABSTRACT

In order to understand hydrogen-induced internal loading on metal, this thesis utilizes CFD (Fluent) software to analyze and simulate the metal system using various parameters including hydrogen diffusion velocity, pressure, concentration and temperature. When the hydrogen diffusion velocity of the boundary condition was set at 0.001 m/s, the analysis and comparisons were done for three metal materials, namely stainless steel (316,314), copper and low-ferritic alloy stainless steel. This result shows that when copper and stainless steel increase their interstitial internal lattice stress at elevated temperature while the low-ferritic alloy stainless steel decreases its stress. When the velocity increases from 0.001 to 0.006 m/s at a fixed temperature of 373K, 873K and 1273K, respectively, the more the velocity increase, the less the stress and internal loading of the stainless steel was observed. The pressure and temperature will be explained in the same time; when the temperature increases the hydrogen atom becomes active, causes mutual collision, and consequently increases the pressure. When the external pressure at the outer surface of the material increases, the relative stress of the hydrogen atom in lattice increases. With respect to the concentration, the simulated concentration from the measured solubility can calculate concentration value, consequently the stress of the material structure can be obtained when the hydrogen enters the material. When hydrogen concentration increases the stress of the hydrogen atom is increased.

Keywords : stress ; simulation ; solubility ; concentration

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## REFERENCES

- [1] 陳維新, 能源工程, 高立圖書有限公司,2008.
- [2] Yu.V. Taran, M.R. Daymond, J. Schreiber, " Interplay of Stresses Induced by Phase Transformation and Plastic Deformation During Cyclic Load of Austenitic Stainless Steel ", Physica B 350,2004,p 98-101.
- [3] T.J. Carter, L.A. Cornish, " Hydrogen in Metals ", Engineering Failure Analysis, Vol.8,2001,p113-121 .
- [4] J. Szilard, R .Haynes, " Ultrasonic Detection of Hydrogen Embrittlement in Steel ", Ultrasonics Symposium,1978, p316-319.
- [5] Ming Au, " High Temperature Electrochemical Charging of Hydrogen and its Application in Hydrogen Embrittlement Research ", Materials Science and Engineering A ,2007, p454-455.

- [6]謝忠霖, “氣與凹槽效應對沃斯田鐵系不銹鋼機械性質之影響”, 國立中央大學材料科學與工程所碩士論文,2007.
- [7]D. Hardie, E.A. Charles, A.H. Lopez, “Hydrogen Embrittlement of High Strength Pipeline Steels”, Corrosion Science 48,2006, p 4378-4385.
- [8]B. R. W. Hinton, R. P. M. Procter, Corros. Sci. 23 (1983), p101.
- [9]K. Farrell, A. G. Quarrel, J. Iron Steel Inst. 202 (1964), p1002.
- [10]R. W. Staehle, J. Hochmann, R.D McCright, J.E Slater, editors. Proceedings of the conference on Stress Corrosion Cracking and Hydrogen Embrittlement of Iron Base Alloys”, Unieux-Firminy,1973.Houston NACE-5, 1977,.
- [11]S. Serbrinsky, E. A Carter, M. Ortiz, “A Quantum-Mechanically Informed Continuum Model of Hydrogen Embrittlement”, Journal of the Mechanics and Physics of Solids 52 ,2004, p2403-2430.
- [12]J. Friedel, Ber. Bunsenges, Physik. Chem. 76, (1972), p 828.
- [13]J. C. Fisher, Acta Metall. 6, 13 (1958) [14]K. W. Keher, in Ref. 1, Vol. I, p. 197.
- [15]R. Gomer, R. Wortman and R. Lundy, J. Chem. Phys. 26, p 1147 (1957).
- [16]M. Wen, S. Fukuyama, K. Yokogawa, “Atomistic simulations of hydrogen effect on dissociation of screw dislocations in nickel”, Scripta Materialia 52, 2005,p 959-962.
- [17]R.A. Oriani, “The physical and metallurgical aspects of hydrogen in metal”, 1993.
- [18]H. G. Fritsche, H. Muller and Ch. Optiz, in Rf. 2, p. 535.
- [19]J. Friedel, Ber. Bunsenges, Physik. Chem. 76, 828 (1972).
- [20]J. C. Fisher, Acta Metall. 6, 13 (1958) [21]K. W. Keher, in Ref. 1, Vol. I, p. 197.
- [22]R.A.Oriani,R.W.Staehle,A. J. Forty, D. Van Roogen, “Hydrogen in metals” Proc. Conf. Fundamental Aspects of SCC, (eds) (NACE) pp 32 – 50(1967) [23]R. K. Dayal and N. Parvathavarthini, Hydrogen Embrittlement in power plant steels, Sadhana Vol.28,parts 3 & 4,June/August 2003,pp.431-451 [24] [http://images.google.com.tw/imgres?imgurl= http://jlnlabs.online.fr/cfr/images/cfr4w35mn.jpg&imgrefurl](http://images.google.com.tw/imgres?imgurl=http://jlnlabs.online.fr/cfr/images/cfr4w35mn.jpg&imgrefurl) [25] <http://www.ttienvinc.com/> [26] <http://cnx.org/content/m15058/latest/> [27] [http://maps.pme.nthu.edu.tw/Manufacturing%20processes/Handouts\\_PDF/ch1.pdf](http://maps.pme.nthu.edu.tw/Manufacturing%20processes/Handouts_PDF/ch1.pdf) [28]陳文照、曾春風、游信和, 材料科學與工程導論,高立圖書有限公司,2005.
- [29]Nettleship, R. Stevens, “Tetragonal Zirconia Polycrystal(TZP)” Int. J. High Technol. Ceram.,3,1987,p 1-32 [30]G.E Kerns, M.T Wang, R.W. Staehle, “Stress Corrosion Cracking and Hydrogen Embrittlement of Iron Base AlloysR.W. Staehle et al.NACE-5,NACH 1977,p.700..
- [31]J. Vo"lkl, G. Alefeld,Hydrogen in Metals I ,Basic Properties. Topics in Applied Physics, Vol. 28. Springer, Berlin(Eds.), 1978.
- [32]謝江琦, “電漿氮離子佈置技術應用於精密塑膠模具機械性質及磨潤性能改善之研究”, 國立成功大學機械工程所碩士論文,2007.
- [33]A.D. LeClaire, Permeation of Gases Through Solids: 2. An Assessment of Measurements of the Steady-State Permeability of H and its Isotopes through Fe, Fe-based Alloys, and Some Commercial Steels. Diffusion Defect Data 34,1983,p 1 – 35.
- [34] <http://corrosion.kaist.ac.kr/> [35]C. San Marchi, B. P. Somerday, S. L. Robinson, Permeability, Solubility and Diffusivity of Hydrogen Isotopes in Stainless Steels at High Gas Pressures, Int J Hydrogen Energy 32 ,2007,p100-116.
- [36] <http://www.efluid.com.cn> [37]CFD Research Corp,CFDRC User Manual,(2003).
- [38]Fluent 6.1 Documentation, User 's Guide [http://www.fluentusers.com,\(2003\)](http://www.fluentusers.com,(2003))。
- [39]劉育成, “矩形LCD製程CVD之熱質傳模擬研究” 國立中山大學機械與電機工程研究所碩士論文,2006.
- [40]J.PVan Doormal, G.D Raithby, “Enhancements of the SIMPLE Method for Predicting Incompressible Fluid Flows”, Numer Heat Transfer,Vol.7,1984,pp.147-163.
- [41]J. Vo"lkl and G. Alefeld, in Hydrogen in Metals I ,Ref. 1,, p. 321.
- [42]E. Wicke and H. Brodowsky, In: G. Alefeld and J. J. Vo"lkl, Editors, Hydrogen in Metals, Vol. II, Springer-Verlag, Berlin 1978, p. 73.
- [43]X. K Sun, J. Xu, Y. Y. Li. Hydrogen Permeation Behaviour in Austenitic Stainless Steels. Mater Sci Eng A114, 1989 ,p 179 – 187.
- [44]M. R Louthan and R. G. Derrick., Hydrogen Transport in Austenitic Stainless Steel . Corros Sci 15 ,1975,p 565-57 [45]H. G. Nelson and J. E. Stein, “Gas-Phase Hydrogen Permeation Through Alpha Iron, 4130 Steel, and 304 Stainless Steel from Less Than 100 to Near 600”, NASA TN D- 7265, NASA,TN D7265, Washington DC, 1973.
- [46]W. Eichenauer, W. Loser and H. Witte., Solubility and Rate of Diffusion of Hydrogen and Deuterium in Nickel and Copper Single Crystals. Z Metallk .56 ,1965,p. 287-293.
- [47]L. Katz, M . Guinan and R. J. Borg. , “Diffusion of H2, D2, and T2 in Single-Crystal Ni and Cu”. Phys Rev B ,vol.4, Issue 2, 1971,p.330-341 [48]G. R. Caskey, A. H. Dexter, M. L. Holzworth, M. R. Louthan and R .G. Derrick., “The Effect of Oxygen on Hydrogen Transport in Copper”. Corrosion 32 ,1976,p.370-374.
- [49]G. R. Caskey, A. H. Dexter, M. L. Holzworth, M. R. Louthan and R.G. Derrick., Hydrogen Transport in Copper (DP-MS-75-6). Savannah River Laboratory, Aiken SC (1975).
- [50]D. R. Begeal. ,Hydrogen and Deuterium Permeation in Copper Alloys, Copper-Gold Brazing Alloys, Gold, and the in Situ Growth of Stable Oxide Permeation Barriers. J Vac Sci Technol 15,1978,p. 1146-1154.
- [51]T. Tanabe, Y. Tamanishi, K. Sawada and S. Imoto. Hydrogen Transport in Stainless Steels. J Nucl Mater 122&123,1984, p.1568-1572.

- [52]J. Xu, X. Z. Yuan, X. K., Sun, B. M. Wei ,Hydrogen Permeation and Diffusion in a 0.2C-13Cr Martensitic Stainless Steel, Scripta Metallurgica et Materialia ,Volume 29, Issue 7,1993, p.925-930.
- [53]N. R. Quick and H. H. Johnson, Acta Metall., 26, 1978, p.903.
- [54]T. P. Perng and C. J. Altstetter, Scrip. Metall., 18, 1984,p.67.
- [55]D.P.Yao,Marster's Thesis, Institute of Metal Research, Academia Sinica,1987, (in Chinese).
- [56]J. Xu , X. K. Sun , Q. Q. Liu, X. Zhao and C. G .Fan ,Hydrogen Permeation Characteristics of Incoloy907 Alloy, Scripa Metallurgica et Materialia, Volume 28, Issue 10, 15 May 1993,p.1251-1256 [57]F. Lecoester, A.M. Brass, J. Che<sup>^</sup>ne, Hydrogen diffusion and Distribution in Alloy 600 and Related Effects Plasticity, 1997.
- [58]T.P. Perng. C. J. Altstetter, Hydrogen Effects in Austenitic Stainless Steels. Vol. 129, 1990, pp. 99-107.
- [59]Y. Adda, and J. Philibert , La Diffusion Dans Les Solides, Presses Universitaires de France, Paris,1966,p.1105-1203.
- [60]C. San Marchi , B. P. Somerday “ Technical Reference on Hydrogen Compatibility of Materials Austenitic Stainless Steel, Sandia National Laboratories,2005.
- [61]M. R. Louthan, G. R. Caskey, J. A. Donovan and D. E. Rawl, Hydrogen Embrittlement of Metals.Mater Sci Eng 10 ,1972, p.357-368.
- [62]B. C. Odegard, J. A. Brooks and A. J. West. The Effect of Hydrogen on Mechanical Behavior of Nitrogen Strengthened Stainless Steel. Effect of Hydrogen on Behavior of Materials, A.W. Thompson and I.M. Bernstein, eds., The Metallurgical Society of AIME, 1976,p.116-125.
- [63]C. San Marchi , B. P . Somerday “ Technical Reference on Hydrogen Compatibility of Materials Low-Alloy Ferritic Steels ” , Sandia National Laboratories,2005.
- [64]E. Mattsson and F. Schueckher. “ An Investigation of Hydrogen Embrittlement in Copper ” . Journal of the Institute of Metals 87 (1958-59) ,p241-247.
- [65]G. R. Caskey, A. H. Dexter, M. L. Holzworth, M. R. Louthan and R.G.Derrick. “ Hydrogen Transportin Copper ” (DP-MS-75-6). Savannah River Laboratory, Aiken SC (1975).
- [66]G. R. Caskey, A. H. Dexter, M. L. Holzworth, M. R. Louthan and R.G. Derrick. “ The Effect of Oxygen on Hydrogen Transport in Copper ” . Corrosion 32 (1976) 370-374.
- [67]J. R. Scully, G. A. Young and S. W. Smith. “ Hydrogen Solubility, Diffusion and Trapping in High Purity Aluminum and Selected Al-base alloys ” . Materials Science Forum 331-337 (2000)1583-1600.
- [68]G. A. Young and J. R. Scully. “ The diffusion and Trapping of Hydrogen in High Purity aluminum ” .Acta Mater 46 (1998) 6337-6349.
- [69]E. Hashimoto and T. Kino. “ Hydrogen diffusion in Aluminum at High Temperatures ” . J P hys F:Met Phys 13 (1983) 1157-1165.17.
- [70]C. San Marchi , B. P. Somerday, “ Technical Reference on Hydrogen Compatibility of Materials pure Aluminum ” , Sandia National Laboratories,2005.
- [71]B. Baranowski, in Hydrogen in Metals II, Vol.29 of Topics in Applied Physics, Edited by G. Alefeld and J. Vo<sup>^</sup>lkl,1978, p. 157.
- [72]R. A. Oriani “ The physical and Metallurgical Aspects of Hydrogen in Metals ” ,(1993)