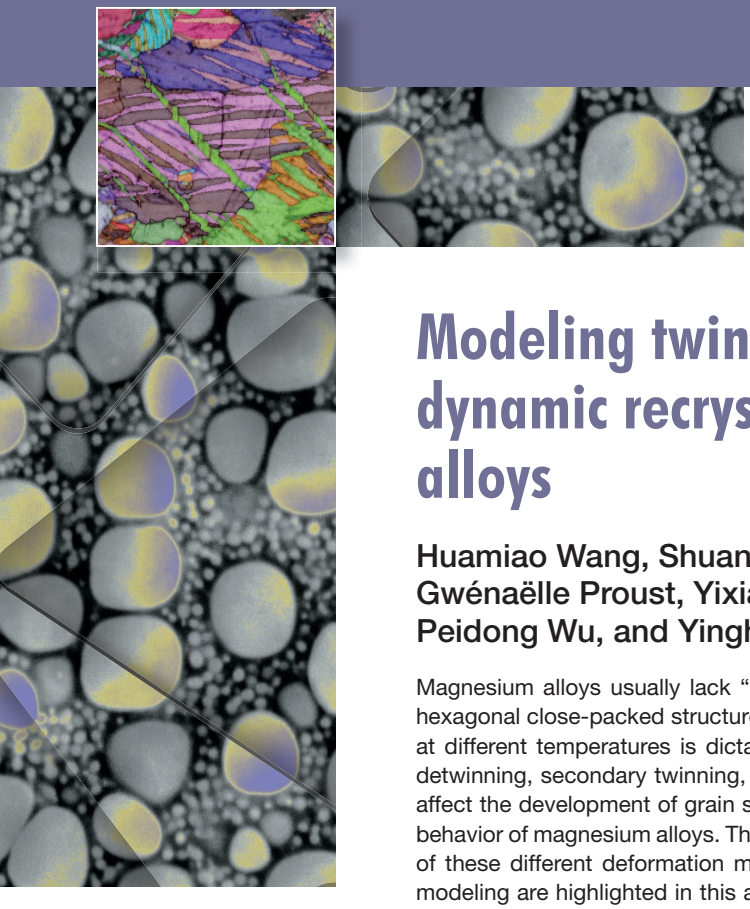


# Modeling twinning, detwinning, and dynamic recrystallization of magnesium alloys

Huamiao Wang, Shuangming Li, Dayong Li, Gwénaëlle Proust, Yixiang Gan, Kun Yan, Ding Tang, Peidong Wu, and Yinghong Peng

Magnesium alloys usually lack "operative deformation slip mechanisms" because of their hexagonal close-packed structure. Therefore, the mechanical behavior of magnesium alloys at different temperatures is dictated by other deformation mechanisms such as twinning, detwinning, secondary twinning, or dynamic recrystallization (DRX). Twinning and DRX can affect the development of grain size and orientation distribution, as well as the deformation behavior of magnesium alloys. The current understanding of the mechanisms and mechanics of these different deformation modes and their implementation in crystal plasticity-based modeling are highlighted in this article. Future directions in the development of constitutive models are also discussed.

## Introduction

Due to their low density, high-specific strength, and stiffness, magnesium (Mg) alloys present a good solution to the increasing demand for lightweight, energy saving, and environmentally friendly engineering systems. Because of their hexagonal close-packed (hcp) crystal structure, Mg alloys show more complex mechanical behavior than other metallic alloys, especially those that are widely available and currently in use.[1,2] Depending on loading conditions such as temperature and strain rate, various deformation mechanisms, including slip, twinning, detwinning, and dynamic recrystallization (DRX), participate to accommodate strain in Mg alloys.

At ambient temperature, in addition to easy basal slip, the alternative mechanisms available are nonbasal slip and tensile twinning.[3,4] The threshold resistance for nonbasal slip is much higher than that for basal slip, hence tensile twinning, whose threshold resistance is close to that of basal slip, becomes an important deformation mechanism for Mg alloys. The hcp structure and twinning activity lead to the characteristic basal texture of wrought Mg alloys, the strong anisotropic ductility and strength, the tension/compression asymmetric stress–strain behavior, and the limited formability at ambient temperature.[5] Upon load reversal during complex loading, detwinning, which is another deformation mechanism, can also occur at room temperature. The alternating twinning and detwinning lead to asymmetric hysteresis stress–strain loops under cyclic loading or lowered yield strength during loading direction change,[6,7] which complicates the understanding and modeling of the mechanical behavior of these alloys.

Hot forming is usually employed for Mg alloy processing because of the improved formability of these alloys at elevated temperatures. A higher temperature generally leads to a lower flow stress, higher ductility/formability, and weaker tension/compression asymmetry,[8–10] which are a result of DRX, nonbasal slip,[11–13] and the suppression of twinning.

Huamiao Wang, School of Mechanical Engineering, Shanghai Jiao Tong University, China; wanghm02@sjtu.edu.cn
Shuangming Li, Northwestern Polytechnical University, China; lsm@nwpu.edu.cn
Dayong Li, School of Mechanical Engineering, Shanghai Jiao Tong University, China; dyli@sjtu.edu.cn
Gwénaëlle Proust, School of Civil Engineering, The University of Sydney, Australia; gwenaelle.proust@sydney.edu.au
Yixiang Gan, School of Civil Engineering, The University of Sydney, Australia; yixiang.gan@sydney.edu.au
Kun Yan, The University of Manchester, UK; kunyan.callaghan@manchester.ac.uk
Ding Tang, School of Mechanical Engineering, Shanghai Jiao Tong University, China; tangding@sjtu.edu.cn
Peidong Wu, Department of Mechanical Engineering, McMaster University, Canada; peidong@mcmaster.ca
Yinghong Peng, School of Materials Science and Engineering, and School of Mechanical Engineering, Shanghai Jiao Tong University, China; yhpeng@sjtu.edu.cn
doi:10.1557/mrs.2019.254

Constitutive modeling is essential for gaining a comprehensive understanding of the behavior of Mg alloys. Atomistic simulations are inadequate to characterize large-scale material behavior because of their limited size and time scales. Crystal plasticity (CP) is a physically based plasticity theory that represents the deformation of a metal at the microscale, which bridges the macroscopic behavior of a polycrystalline aggregate to the deformation mechanisms at the scale of the grains.[14,15] Full-field approaches, such as the CP finite element (CPFE) method,[16] account explicitly not only for grain morphology and the interaction between a grain and its neighbors, but also for the heterogeneous deformation. Due to their computational efficiency, mean-field approaches that employ certain homogenization methods are also widely applied to study the response of a polycrystal. The Taylor[17] and self-consistent[18] methods are popular examples.

The CP models provide the platform to incorporate deformation mechanisms. Early models consider slip as the major plastic deformation mechanism. This article highlights progress in modeling twinning, detwinning, and DRX for Mg alloys.

## Twinning

Twinning usually occurs sequentially in terms of twin nucleation (TN), twin propagation, and twin growth when stretching the Mg alloy along its *c*-axis or loading equivalently. The accommodation of finite shear deformation and abrupt lattice reorientation could contribute to both the ductility and the strength of Mg alloys. Recent studies using atomistic simulations have shed valuable light on understanding the atomistic mechanisms associated with deformation twinning.[19,20] Extensive experimental observations and atomistic simulations have revealed that twins preferentially nucleate at local inhomogeneities, mostly at grain boundaries (GBs).[21,22] TN models developed based on the statistical distribution of GB dislocations effectively describe the important influence of local stresses near GB area on TN.[23] Many models focus more on twin growth, and the associated reorientation and work hardening.[23,24] Handling the extremely large number of new orientations is difficult to address by twinning schemes.

The volume fraction transfer (VFT) scheme[18] partitions the Euler space into a fixed number of discrete cells with appropriate weights to represent the texture of samples. The VFT scheme robustly accounts for the contribution to texture of every twinning system in every grain by transferring twin volume fractions (TVFs) from one cell to another. The main drawback is that the "grain" identity is lost, and the implementation of a realistic hardening scheme is not allowed.

The predominant twin reorientation (PTR) scheme treats twinning as a pseudo-slip mechanism and tracks the evolution of the TVF.[15,23,24] A grain with TVF reaching a threshold value is completely reoriented into its predominant twin orientation. The threshold value depends statistically on the total TVF in the entire polycrystal to ensure that heavily twinned grains are reoriented. This scheme has been applied intensively to study the twinning behavior of Mg alloys.[25,26] The major advantage is that the number of total grain orientations remains constant. However, multiple twinning variants can be simultaneously active in a grain, which cannot be predicted by the PTR scheme.

Kalidindi's twin scheme allows tracking the evolution of multiple twinning systems in each grain.[27] The orientation of a twinned region is obtained according to the matrix–twin crystallographic relation that has mirror symmetry with respect to the twin boundary. The soundness of tracking multiple twinning systems and slip in both twinned and untwinned regions has been acknowledged by researchers, and the model has been applied to study the plasticity of hcp materials.[28,29] The disadvantage is the cumbersome implementation into the CP framework when taking accounting for the slip in twinned regions and the increase in the number of grains.

A twin nucleation, propagation, and growth model that explicitly takes into account the stress relaxation associated with twin initiation and propagation has also been developed (**Figure 1**).[30,31] This model relies on the fact that the resistance to twin growth is less than or equal to that for twin initiation.[3] It has been rationalized that the stress relaxation drives a just-nucleated twin to propagate, while work hardening promotes twin growth after its propagation. The model demonstrates the processes of twin nucleation, propagation, growth, and transmission across GBs.[31,32]

## Detwinning

Subjected to strain path change, Mg alloys often undergo detwinning subsequent to twinning, which necessitates the model to handle both phenomena. The composite grain model, which treats twins as parallel lamellae, allows for detwinning, but it only takes into account the predominant

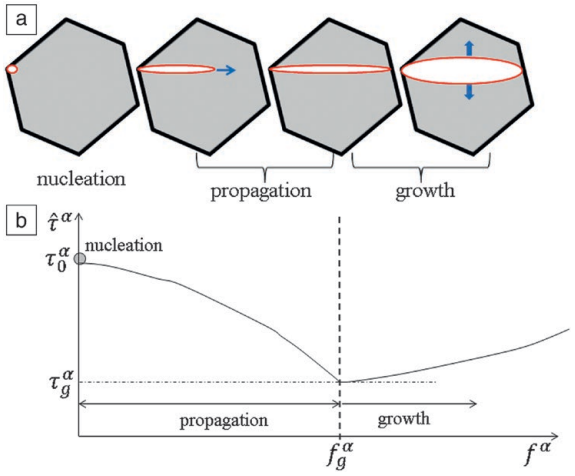



**Figure 1.** Schematic representations of (a) twin nucleation, propagation, and growth in a grain, and (b) resistance to twin nucleation, propagation, and growth.[30] Note: $\hat{\tau}^\alpha$, twinning resistance; $f^\alpha$, twin volume fraction. At nucleation, the resolved shear stress must overcome a high resistance, $\tau_0^\alpha$. During twin propagation, the resistance to twinning decreases to its minimum $\tau_g^\alpha$ at the twin volume fraction, $f^\alpha = f_g^\alpha$.

twinning system.[28] The twinning and detwinning (TDT) model acknowledges and approximates the key fact that the stress on the twin boundary (TB) drives the twins.[33] Consequently, mechanisms for twin initiation (which comprises twin nucleation and propagation) and twin growth are introduced for twinning, while mechanisms for twin shrinkage and retwinning (twinning of a twinned region) model detwinning.[33,34] The TDT model can simulate twinning and detwinning behaviors in hcp metals and capture key features such as texture evolution and hardening behavior.[35–39] Secondary twinning occurs when the retwinning variant is not the same as the one that created the twin in the first place. The most frequently observed $\{10\bar{1}1\}$–$\{10\bar{1}2\}$ double twin structure is a particular type of secondary twinning, which may cause rapid flow localization and failure in Mg alloys.[40,41] The TDT model has been extended to account for and demonstrate the nontrivial role of secondary twinning behavior under complex loading conditions.[42]

## Dynamic recrystallization

Discontinuous DRX (DDRX) and continuous DRX (CDRX) are important DRX mechanisms for Mg alloys at high temperatures. These mechanisms generate new grains that alter the microstructure and mechanical behavior of the alloys. The nucleation of recrystallized grains and the long-range migration of GBs are two major features of DDRX.[43,44] A DDRX scheme has been proposed to correlate the nucleation probability to the loading rate, GB area, and temperature once a critical dislocation density has been reached.[10] The growth of the nucleated grains is determined by the GB mobility and relative difference in dislocation density across the GB. The results of simulations, realized at different temperatures, with respect to plastic deformation, grain orientation, and grain size, are a reflection of the low flow stress, high ductility, and weak anisotropy associated with Mg alloys at higher temperatures (**Figure 2**).

CDRX is favorable for fine-grained Mg alloys at elevated temperatures ranging from 200°C to 450°C. New grains are generated by the continuous increase in misorientation inside a given grain, which leads to the development of high-angle grain boundaries (HAGBs) without obvious GB migration.[44,45] These characteristics have been described in the CDRX scheme, where the misorientation between the core and boundary of a grain is tracked through lattice distortion.[46] Once the misorientation reaches a critical value, HAGBs form and new grains are born. Contrary to DDRX, the growth of grains generated from CDRX is negligible.

## Future directions

Some recent experimental findings need to be implemented in the CP models. For example, CP-based models view twins as two-dimensional (2D) domains. Recently, the three-dimensional structure of twins has been characterized, and the growth and structure along the lateral direction were found to be different from those developed from the 2D point of view.[47] Additionally, twin–twin interactions and junctions, also not accounted for in any model, influence the hardening behavior of Mg alloys.[7] The failure in predicting the internal stresses demands better characterization of the stress state of newly created twins.[36] It has been shown that twin pairs form when a twin crosses the GB, which affects the macroscopic behavior. GB sliding, a deformation mechanism that involves displacement of grains against each other, is another important mechanism of Mg alloy deformation at a high temperature, especially when the grain size is below the submicrometer scale. The quantitative description of the entities previously mentioned and their implementation into mesoscale material models are still lacking and are good areas for future work.

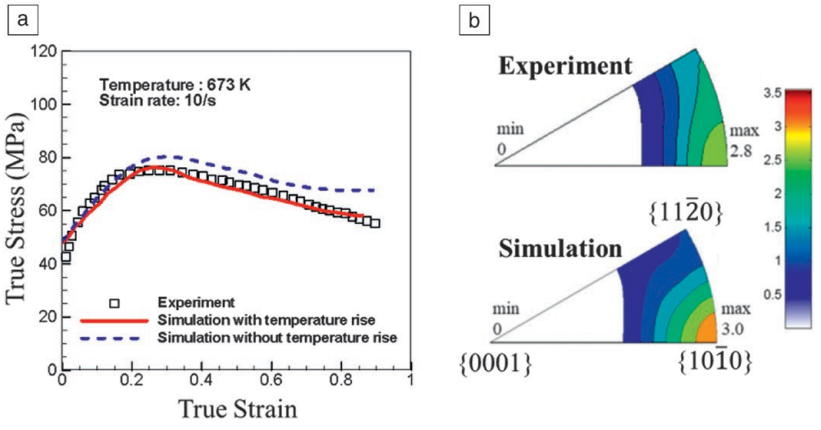



**Figure 2.** Experimental and predicted (a) stress–strain curves at a strain rate of 10 per s and a temperature of 673 K and (b) textures at a strain of 0.9 shown in terms of the inverse pole figures.[10] Note that temperature rises with loading at a high strain rate. Better agreement with experimental results was obtained if the temperature rise was considered. The inverse pole figures were obtained through a stereographic projection to reflect the distribution of the grain orientations. Both experimental and simulation results revealed that the $\{10\bar{1}0\}$ crystal directions were developed preferentially along the loading direction.

## Acknowledgments

H.W. was supported by the Shanghai Pujiang Program (18PJ1405000), the Foundation of State Key Laboratory of Solidification Processing (SKLSP201810), and the National Natural Science Foundation of China (No. 51975365). D.L. was supported by the National Natural Science Foundation of China (No. 51675331). P.W. was supported by the Natural Sciences and Engineering Research Council of Canada. The authors acknowledge the support from The University of Sydney-Shanghai Jiao Tong University Partnership Collaboration Awards. K.Y. is supported by the Diamond Manchester Collaboration.

## References

1. T.M. Pollock, *Science* **328**, 986 (2010).
2. G. Proust, *Science* **364**, 30 (2019).

3. J.W. Christian, S. Mahajan, *Prog. Mater. Sci.* **39**, 1 (1995).
4. Q. Yu, Y. Jiang, J. Wang, *Scr. Mater.* **96**, 41 (2015).
5. C.S. Roberts, *Magnesium and Its Alloys* (Wiley, New York, 1960).
6. X.Y. Lou, M. Li, R.K. Boger, S.R. Agnew, R.H. Wagoner, *Int. J. Plast.* **23**, 44 (2007).
7. Q. Yu, J.X. Zhang, Y.Y. Jiang, *Philos. Mag. Lett.* **91**, 757 (2011).
8. A. Jain, S.R. Agnew, *Mater. Sci. Eng. A* **462**, 29 (2007).
9. T. Al-Samman, X. Li, *Mater. Sci. Eng. A* **527**, 3450 (2010).
10. T. Tang, G. Zhou, Z. Li, D. Li, L. Peng, Y. Peng, P. Wu, H. Wang, M.G. Lee, *Int. J. Plast.* **116**, 159 (2019).
11. T. Al-Samman, K.D. Molodov, D.A. Molodov, G. Gottstein, S. Suwas, *Acta Mater.* **60**, 537 (2012).
12. N. Stanford, M.D. Callaghan, B. de Jong, *Mater. Sci. Eng. A* **565**, 459 (2013).
13. X. Liu, J.J. Jonas, L.X. Li, B.W. Zhu, *Int. J. Plast.* **27**, 1916 (2013).
14. R.J. Asaro, A. Needleman, *Acta Metall.* **33**, 923 (1985).
15. C.N. Tomé, R.A. Lebensohn, U.K. Kocks, *Acta Metall. Mater.* **39**, 2667 (1991).
16. P.R. Dawson, S.R. MacEwen, P.D. Wu, *Int. Mater. Rev.* **48**, 86 (2003).
17. G.I. Taylor, *J. Inst. Met.* **62**, 307 (1938).
18. R.A. Lebensohn, C.N. Tomé, *Acta Metall. Mater.* **41**, 2611 (1993).
19. J. Wang, J.P. Hirth, C.N. Tomé, *Acta Mater.* **57**, 5521 (2009).
20. J. Wang, I.J. Beyerlein, C.N. Tomé, *Int. J. Plast.* **56**, 156 (2014).
21. I.J. Beyerlein, L. Capolungo, P.E. Marshall, R.J. McCabe, C.N. Tomé, *Philos. Mag.* **90**, 2161 (2010).
22. S.R. Niezgoda, A.K. Kanjarla, I.J. Beyerlein, C.N. Tomé, *Int. J. Plast.* **56**, 119 (2014).
23. P. Van Houtte, *Acta Metall. Mater.* **26**, 591 (1978).
24. C.N. Tomé, P.J. Maudlin, R.A. Lebensohn, G.C. Kaschner, *Acta Mater.* **49**, 3085 (2001).
25. S.R. Agnew, O. Duygulu, *Int. J. Plast.* **21**, 1161 (2005).
26. H. Wang, B. Raeisinia, P.D. Wu, S.R. Agnew, C.N. Tomé, *Int. J. Solids Struct.* **47**, 2905 (2010).
27. S.R. Kalidindi, *J. Mech. Phys. Solids* **46**, 267 (1998).
28. G. Proust, C.N. Tomé, G.C. Kaschner, *Acta Mater.* **55**, 2137 (2007).
29. G. Proust, C.N. Tomé, A. Jain, S.R. Agnew, *Int. J. Plast.* **25**, 861 (2009).
30. P.D. Wu, X.Q. Guo, H. Qiao, D.J. Lloyd, *Mater. Sci. Eng. A* **625**, 140 (2015).
31. H. Qiao, M.R. Barnett, P.D. Wu, *Int. J. Plast.* **86**, 70 (2016).
32. R. Xin, Z. Liu, Y. Sun, H. Wang, C. Guo, W. Ren, Q. Liu, *Int. J. Plast.* (2019), doi:10.1016/j.ijplas.2019.07.018.
33. H. Wang, P.D. Wu, C.N. Tomé, J. Wang, *Mater. Sci. Eng. A* **555**, 93 (2012).
34. H. Wang, P.D. Wu, J. Wang, C.N. Tomé, *Int. J. Plast.* **49**, 36 (2013).
35. X.Q. Guo, W. Wu, P.D. Wu, H. Qiao, K. An, P.K. Liaw, *Scr. Mater.* **69**, 319 (2013).
36. H. Qiao, S.R. Agnew, P.D. Wu, *Int. J. Plast.* **65**, 61 (2015).
37. H. Wang, B. Clausen, L. Capolungo, I.J. Beyerlein, J. Wang, C.N. Tomé, *Int. J. Plast.* **79**, 275 (2016).
38. H. Wang, P.D. Wu, S. Kurukuri, M.J. Worswick, Y. Peng, D. Tang, D. Li, *Int. J. Plast.* **107**, 207 (2018).
39. C. Ma, H. Wang, T. Hama, X. Guo, X. Mao, J. Wang, P.D. Wu, *Int. J. Plast.* **121**, 261 (2019).
40. Q. Ma, H. El Kadiri, A.L. Oppedal, J.C. Baird, M.F. Horstemeyer, M. Cherkaoui, *Scr. Mater.* **64**, 813 (2011).
41. S. Niknejad, S. Esmaeili, N.Y. Zhou, *Acta Mater.* **102**, 1 (2016).
42. H. Qiao, X.Q. Guo, S.G. Hong, P.D. Wu, *J. Alloys Compd.* **725**, 96 (2017).
43. R.D. Doherty, *Prog. Mater. Sci.* **42**, 39 (1997).
44. T. Sakai, A. Belyakov, R. Kaibyshev, H. Miura, J.J. Jonas, *Prog. Mater. Sci.* **60**, 130 (2014).
45. C.H. Park, C.-S. Oh, S. Kim, *Mater. Sci. Eng. A* **542**, 127 (2012).
46. G. Zhou, Z. Li, D. Li, Y. Peng, H. Wang, P.D. Wu, *Mater. Sci. Eng. A* **730**, 438 (2018).
47. Y. Liu, N. Li, S. Shao, M. Gong, J. Wang, R.J. McCabe, Y. Jiang, C.N. Tomé, *Nat. Commun.* **7**, 11577 (2016). □

**Huamiao Wang** is an associate professor in the School of Mechanical Engineering at Shanghai Jiao Tong University (SJTU), China. He received his BSc, MSc, and PhD degrees from Xi'an Jiao Tong University, China, Tsinghua University, China, and McMaster University, Canada, respectively. He was a research associate at McMaster University and Los Alamos National Laboratory from 2011 to 2017 and joined SJTU in 2017. His research interests focus on the field of the mechanics of engineering materials, specifically in multiscale modeling, and machine learning-based manufacturing, regulating, and controlling processes. Wang can be reached by email at wanghm02@sjtu.edu.cn.

**Shuangming Li** has been a professor of materials processing at Northwestern Polytechnical University (NWPU), China, since 2005. He received his PhD degree in 1999 from NWPU and joined the Harbin Institute of Technology, China, as a postdoctoral fellow. He joined the State Key Laboratory of Solidification Processing at NWPU in 2001. His research focuses on metals solidification, superalloys, and single-crystal growth for structure-functional related applications. He has published more than 100 peer-reviewed journal papers and supervised more than 40 graduate students. Li can be reached by email at lsm@nwpu.edu.cn.

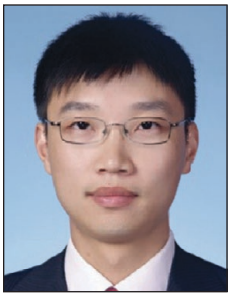
**Dayong Li** is a full professor in the School of Mechanical Engineering at Shanghai Jiao Tong University, China. He received his PhD degree in solid mechanics from Jilin University of Technology, China, in 2000. His research interests include crystal plasticity, metal forming, and materials strength. Li has published more than 100 journal papers and served as a peer reviewer for more than 10 journals. His awards include the Innovation Award of Shanghai International Industrial Expo, China, in 2015, and a Science and Technology Progress Award of China in 2014. Li can be reached by email at dyli@sjtu.edu.cn.

**Gwénaëlle Proust** is an associate professor in the School of Civil Engineering at The University of Sydney, Australia. She received her PhD degree from Drexel University in materials science and engineering in 2005. Her research focuses on understanding the relationships between materials properties and microstructures to improve material performance. Her current research includes investigating and modeling the effects of mechanical deformation on microstructure evolution of metals to gain an understanding of the effects of complex loading on the mechanical response of materials. Proust can be reached by email at gwenaelle.proust@sydney.edu.au.

**Yixiang Gan** has been a senior lecturer in the School of Civil Engineering at The University of Sydney, Australia, since 2010. He received his Dr-Ing degree in mechanical engineering from the Karlsruhe Institute of Technology (KIT), Germany, in 2008, and his BE/BBA and ME degrees from Xi'an Jiaotong University, China, in 2002 and 2005, respectively. He was a research scientist at KIT, conducting research on several European projects on nuclear fusion. His research interests include the mechanics of materials, especially granular and porous media, multiphase flow, the mechanics of interfaces, and heat and electrical conduction. Gan can be reached by email at yixiang.gan@sydney.edu.au.

**Kun Yan** is a research fellow at the Diamond Light Source and The University of Manchester, UK. She completed postdoctoral research at the Australian Nuclear Science and Technology Organisation and the University of Wollongong, Australia. Her research includes the plastic deformation mechanisms of thermomechanical processed high-manganese steels, including twinning-induced and transformation-induced plasticity steel. Her current research focuses on damage formation and modeling of multiphase materials utilizing advanced synchrotron radiation x-ray tomography and diffraction techniques. Yan can be reached by email at kunyan.callaghan@manchester.ac.uk.

**Peidong Wu** has been a professor in the Department of Mechanical Engineering at McMaster University, Canada, since 2006. He received his BSc, MSc, and PhD degrees from Zhejiang University, China, China University of Mining and Technology, and Delft University of Technology, The Netherlands, respectively. He conducted research at Alcan International Limited, Research and Development Centre in 1997. Wu's awards include a Canada International Fellowship by the Natural Sciences and Engineering Research Council in 1994, and the International Journal of Plasticity Medal in 2009. His research focuses on the mechanics of engineering materials. Wu can be reached by email at peidong@mcmaster.ca.



**Ding Tang** has been an associate professor in the School of Mechanical Engineering at Shanghai Jiao Tong University (SJTU), China, since 2011. He received his BSc and MSc degrees from Central South University, China, and his PhD degree from SJTU. His research interests focus on the field of the plastic forming technology, microchannel tube forming, multiscale modeling and machine learning-based manufacturing. Tang can be reached by email at tangding@sjtu.edu.cn.

**Yinghong Peng** is a distinguished professor in the School of Materials Science and Engineering, and the School of Mechanical Engineering at Shanghai Jiao Tong University (SJTU), China. He is currently the director of the Institute of Mechatronics Design and Knowledge-Based Engineering at SJTU. He is also the program director for the National Research Foundation of Singapore's CREATE Program of "Energy and Environmental Sustainability Solutions for Megacities." His research focuses on integrated computational materials engineering and knowledge-based engineering technology in the mechatronics design field. Peng can be reached by email at yhpeng@sjtu.edu.cn.