


## 2-1. IROAST Distinguished Professors

No.	Name	Project Title
2-1-1	<b>U. Rajendra ACHARYA</b> University of Southern Queensland (Australia)	Artificial Intelligence in Healthcare
2-1-2	<b>Dmitri Aleks MOLODOV</b> RWTH Aachen University (Germany)	Mechanics and dynamics of grain boundaries in Al and Mg bicrystals
2-1-3	<b>László PUSZTAI</b> Wigner Research Centre for Physics (Hungary)	Nanoscale assemblies in hydrogen-bonded liquids and in amorphous materials
2-1-4	<b>Yufeng ZHENG</b> School of Materials Science and Engineering, Peking University (China)	Development and management of biomaterials

## FY2023 IROAST Research Activity Annual Report–Distinguished Professor

No. 2-1-1	Artificial Intelligence in Healthcare			
Name	U. Rajendra ACHARYA	Title	Professor	
Affiliation	University of Southern Queensland, Australia Email: <a href="mailto:Rajendra.Acharya@unisq.edu.au">Rajendra.Acharya@unisq.edu.au</a>			
Research Field	Data science and AI			
Period of appointment	April 1, 2023- March 31, 2024			
Host Professor	Makiko KOBAYASHI			
Affiliation	Faculty of Advanced Science and Technology Email: <a href="mailto:kobayashi@cs.kumamoto-u.ac.jp">kobayashi@cs.kumamoto-u.ac.jp</a>	Title	Professor	

### Research achievements

- 1) Symposiums/seminars for graduate students/undergraduate students during stay in KU from 25<sup>th</sup> September to 2<sup>nd</sup> October.



(The 100<sup>th</sup> IROAST Seminar on Sep. 29, 2023)

- 2) Academic research papers published from 2023/4 to 2024/3
  1. Novel tiny textural motif pattern-based RNA virus protein sequence classification model, Mehmet Erten, Emrah Aydemir, Prabal Datta Barua, Mehmet Baygin, Sengul Dogan, Turker Tuncer, Ru-San Tan, Abdul Hafeez-Baig, U. Rajendra Acharya, Expert Systems with Applications 242, 122781, 2024  
<https://doi.org/10.1016/j.eswa.2023.122781>  
*\*Scheduled to be issued in May 2024*
  2. GCLP: An automated asthma detection model based on global chaotic logistic pattern using cough sounds, Kilic, Mehmet; Barua, Prabal Datta; Keles, Tugce; Yildiz, Arif Metehan; Tuncer, Ilknur; Dogan, Sengul; Baygin, Mehmet; Tuncer, Turker; Kuluozturk, Mutlu; Tan, Ru-San; Acharya, U. Rajendra, Engineering Applications of Artificial Intelligence, 127, Part A, 107184, 2024  
<https://doi.org/10.1016/j.engappai.2023.107184>
  3. A Novel Attention-Based Model for Semantic Segmentation of Prostate Glands Using Histopathological Images, Mahesh Anil Inamdar; U. Raghavendra; Anjan Gudigar; Sarvesh Bhandary; Massimo Salvi; Ravinesh C. Deo; Prabal Datta Barua; Edward J. Ciaccio; Filippo Molinari; U. Rajendra Acharya, IEEE Access 11, 108982-108994 (2023)  
<https://doi.org/10.1109/ACCESS.2023.3321273>

4. FF-BTP Model for Novel Sound-Based Community Emotion Detection, Arif Metehan Yildiz, Masayuki Tanabe, Makiko Kobayashi, Ilknur Tuncer, Prabal Datta Barua, Sengul Dogan, Turker Tuncer, Ru San Tan, U. Rajendra Acharya, IEEE Access 11, 108705-108715 (2023)  
<https://doi.org/10.1109/ACCESS.2023.3318751>
5. Innovative Fibromyalgia Detection Approach Based on Quantum-Inspired 3LBP Feature Extractor Using ECG Signal, Prabal Datta Barua, Makiko Kobayashi, Masayuki Tanabe, Mehmet Baygin, Jose Kunnel Paul, Thomas Iype, Sengul Dogan, Turker Tuncer, Ru San Tan, U. Rajendra Acharya, IEEE Access 11, 101359-101372 (2023)  
<https://doi.org/10.1109/ACCESS.2023.3315149>
6. Brain tumor detection and screening using artificial intelligence techniques: Current trends and future perspectives, Raghavendra, U.; Gudigar, Anjan; Paul, Aritra; Goutham, T. S.; Inamdar, Mahesh Anil; Hegde, Ajay; Devi, Aruna; Ooi, Chui Ping; Deo, Ravinesh C.; Barua, Prabal Datta; Molinari, Filippo; Ciaccio, Edward J.; Acharya, U. Rajendra, Computers in Biology and Medicine 163, 107063 (2023)  
<https://doi.org/10.1016/j.compbiomed.2023.107063>
7. Automated detection of scaphoid fractures using deep neural networks in radiographs, Amanpreet Singh, Ali Abbasian Ardakani, Hui Wen Loh, P. V. Anamika, U. Rajendra Acharya, Sidharth Kamath, Anil K. Bhat, Engineering Applications of Artificial Intelligence, 122, 106165, 2023  
<https://doi.org/10.1016/j.engappai.2023.106165>
8. Automated detection and screening of depression using continuous wavelet transform with electroencephalogram signals, U. Raghavendra, Anjan Gudigar, Yashas Chakole, Praneet Kasula, D. P. Subha, Nahrizul Adib Kadri, Edward J. Ciaccio, U. Rajendra Acharya, Expert Systems 40 (4), e12803 (2023)  
<https://doi.org/10.1111/exsy.12803>
9. A Data-Driven Hybrid Methodology Using Randomized Low-Rank DMD Approximation and Flat-Top FIR Filter for Voltage Fluctuations Monitoring in Grid-Connected Distributed Generation Systems, Mohan, Neethu; Kumar, S. Sachin; Soman, K. P.; Sujadevi, V. G.; Poornachandran, Prabakaran; Acharya, U. Rajendra, IEEE Access 11, 39228 - 39242, 2023  
<https://doi.org/10.1109/ACCESS.2023.3267125>
10. SchizoNET: a robust and accurate Margenau–Hill time-frequency distribution based deep neural network model for schizophrenia detection using EEG signals, Smith K Khare, Varun Bajaj and U Rajendra Acharya, Physiological Measurement 44, 3, 035005 (2023)  
<https://doi.org/10.1088/1361-6579/acbc06>  
*\*Published in the previous year, but included in this report due to being unlisted in the previous year.*
11. Automated detection of airflow obstructive diseases: A systematic review of the last decade (2013-2022), Shuting Xu, Ravinesh C Deo, Jeffrey Soar, Prabal Datta Barua, Oliver Faust, Nusrat Homaira, Adam Jaffe, Arm Luthful Kabir, U Rajendra Acharya, Computer Methods and Programs in Biomedicine 241, 107746, 2023  
<https://doi.org/10.1016/j.cmpb.2023.107746>

12. An explainable and interpretable model for attention deficit hyperactivity disorder in children using EEG signals, Smith K Khare, U Rajendra Acharya, Computers in Biology and Medicine 155, 106676 (2023)

<https://doi.org/10.1016/j.combiomed.2023.106676>

*\*Published in the previous year, but included in this report due to being unlisted in the previous year.*

13. Automated warfarin dose prediction for Asian, American, and Caucasian populations using a deep neural network, Jahmunah, V.; Chen, Sylvia; Oh, Shu Lih; Acharya, U. Rajendra; Chowbay, Balram, Computers in Biology and Medicine, 153, 106548, 2023

<https://doi.org/10.1016/j.combiomed.2023.106548>

*\*Published in the previous year, but included in this report due to being unlisted in the previous year.*

14. An Explainable Deep Learning Model to Prediction Dental Caries Using Panoramic Radiograph Images, Oztekin, Faruk; Katar, Oguzhan; Sadak, Ferhat; Yildirim, Muhammed; Cakar, Hakan; Aydogan, Murat; Ozpolat, Zeynep; Yildirim, Tuba Talo; Yildirim, Ozal; Faust, Oliver; Acharya, U. Rajendra, Diagnostics, 13 (2), 226, 2023

<https://doi.org/10.3390/diagnostics13020226>

*\*Published in the previous year, but included in this report due to being unlisted in the previous year.*


15. Uncertainty quantification in DenseNet model using myocardial infarction ECG signals, Jahmunah, V.; Ng, E. Y. K.; Tan, Ru-San; Oh, Shu Lih; Acharya, U. Rajendra, Computer Methods and Programs in Biomedicine, 229, 107308, 2023

<https://doi.org/10.1016/j.cmpb.2022.107308>

*\*Published in the previous year, but included in this report due to being unlisted in the previous year.*

3) Implementation and progress of international joint research between KU and UniSQ, Australia

## FY2023 IROAST Research Activity Annual Report–Distinguished Professor

No. 2-1-2	Mechanics and dynamics of grain boundaries in Al and Mg bicrystals			
Name	Dmitri A. MOLODOV	Title	Professor	
Affiliation (home)	Institute of Physical Metallurgy and Materials Physics (IMM), RWTH Aachen University, Germany Email: molodov@imm.rwth-aachen.de			
Research Field	Advanced materials			
Period of appointment	April 1, 2023- March 31, 2024			
Host Professor	Sadahiro TSUREKAWA			
Affiliation	Faculty of Advanced Science and Technology Email: turekawa@kumamoto-u.ac.jp	Title	Professor	

### Details of Activities

(i) Symposia/seminars for graduate students/undergraduate students in KU:

The two lectures on the topic of "Grain Boundary Migration" were held on May 16 and 18, 2023 (90 minutes each) for graduate students in the framework of the regular class of Professor Tsurekawa "Materials Interface Science".

※The details of these seminar are shown in a report of seminar (4-2 IROAST seminars)

(ii) In the beginning of the reporting period, our research within the four-year project to study the plasticity and dynamic recrystallization of Mg single crystals was successfully completed. The most important recent observations in this work can be summarized as follows. Crystals of 'hard' orientations compressed along the c-axis exhibited limited room temperature ductility, although pyramidal  $\langle c+a \rangle$  slip was readily activated. In the case of orientations favorably aligned for c-axis extension, profuse  $\{10\bar{1}2\}$  extension twinning was the primary mode of incipient deformation. In both cases of compression along  $\langle 11\bar{2}0 \rangle$  and  $\langle 10\bar{1}0 \rangle$  directions,  $\{10\bar{1}2\}$  extension twins completely converted the starting orientations into twin orientations; the subsequent deformation behavior of the differently oriented crystals, however, was remarkably different. Prismatic slip was not found to operate at room temperature in the case of starting orientations most favorably aligned for prismatic slip; instead, cooperative  $\{10\bar{1}2\}$  extension and  $\{10\bar{1}1\}$  contraction twinning was activated. A two-stage work hardening behavior was observed in 'soft' Mg crystals aligned for single or coplanar basal slip. The higher work hardening in the second stage was attributed to changes in the microstructure rather than the interaction of primary dislocations with forest dislocations. In the resulting manuscript the mentioned experimental findings were critically discussed and compared with the results of our previous work as well as existing knowledge from the literature.

The paper, which provides an overview on the deformation behavior and microstructure evolution of Mg crystals under plane strain compression, was published in the open access journal Metals:

Konstantin D. Molodov, Talal Al-Samman, Dmitri A. Molodov: On the Plasticity and deformation mechanisms in magnesium crystals, Metals, 2023, 13(4), 640.

<https://doi.org/10.3390/met13040640>.

(iii) During the reporting period we have also continued the experimental study of the response of grain boundaries to deformation, particularly with respect to how they accommodate deformation induced lattice rotation of adjoining crystallites by changing their structure and geometry. In a series of experiments the deformation behaviour of Mg bicrystals with  $90^\circ\langle 11\bar{2}0\rangle$  symmetric tilt boundary, strained in plane-strain compression up to different final strains at the ambient temperature, was addressed. Due to the initial soft orientation of the two crystals, activation of basal slip in each crystal gave rise to lattice rotation around the transverse direction towards the compression direction of the channel-die. The grain boundary character was measured to change dramatically during plastic strain. At larger strains the presence of the boundary resulted in the pronounced lattice curvature in the crystals regions in the vicinity of the boundary. Hundreds of single EBSD maps with a small step size were obtained from the GB region and stitched together to produce large panoramic maps of a macroscopic scale. Although very time-consuming, this technique has proven useful in clarifying the origin of the non-uniform deformation zones in the vicinity of the grain boundary and explains the mechanisms, by which the grain boundary was able to cope with the imposed strain before fracture. Interestingly, several variants of extension twins were observed as an additional deformation mechanism despite having negative Schmid factors. Systematic investigation of their resulting combined shear components with respect to the sample coordinate system revealed an alignment along the longitudinal direction of the channel-die, therefore justifying their nucleation.

Furthermore, the deformation mechanisms and dynamic recrystallization (DRX) behavior of Mg bicrystals with a symmetric  $90^\circ\langle 10\bar{1}0\rangle$  and a  $90^\circ\langle 11\bar{2}0\rangle$  tilt grain boundaries, were investigated under deformation at  $200^\circ\text{C}$  and  $400^\circ\text{C}$ . Again, as at room temperature, the existence of the grain boundary gave rise to dislocation pile-up in its vicinity, leading to much larger TD lattice rotations within the boundary region compared to the bulk. With increasing temperature, the deformation was generally more uniform towards the bulk due to enhanced dislocation mobility and more uniform stress distribution. Dynamic recrystallization at  $200^\circ\text{C}$  was initiated in  $\{10\bar{1}1\}$  compression twins at strains of 40% and higher. At  $400^\circ\text{C}$ , DRX consumed the entire grain boundary region and gradually replaced the deformed microstructure with progressing deformation.

The results obtained and their analysis were reported in the papers published in the Journal of Magnesium and Alloys, and Crystals:

Kevin Bissa, Talal Al-Samman, Dmitri A. Molodov: Deformation behavior of magnesium bicrystals with symmetrical  $90^\circ\langle 11\bar{2}0\rangle$  tilt grain boundaries analyzed by large area EBSD mapping, Journal of Magnesium and Alloys, 2023, v. 11, no. 5, pp. 1556-1566.

<https://doi.org/10.1016/j.jma.2023.03.009>.

Kevin Bissa, Talal Al-Samman, Dmitri A. Molodov: High temperature deformation and recrystallization behavior of magnesium bicrystals with  $90^\circ\langle 10\bar{1}0\rangle$  and  $90^\circ\langle 11\bar{2}0\rangle$  tilt grain boundaries, Journal of Magnesium and Alloys, 2024, v. 12, no. 2, pp. 625-638.

<https://doi.org/10.1016/j.jma.2024.01.021>.

Kevin Bissa, Talal Al-Samman, Dmitri A. Molodov: On melt growth and microstructure characterization of magnesium bicrystals, Crystals, 2024, 14, 130.

<https://doi.org/10.3390/cryst14020130>.

(iv) The other focus of our research in the reporting period was put on the investigation of the migration behaviour of different grain boundaries with misorientations close to the  $\Sigma 3$  CSL orientation relationship in high purity Al bicrystals. The boundary behaviour was examined under the action of a capillary driving force and an applied mechanical stress. The experiments were performed by an *in-situ* technique to observe and measure the boundary migration with a

scanning electron microscope. Molecular statics (MS) computer simulations were performed to analyze the effect of the inclination dependence of grain boundary energy on the faceting behavior of nearly  $\Sigma 3$  grain boundaries. An analysis of the behavior of the nearly  $\Sigma 3$   $60^\circ\langle 111 \rangle$  incoherent  $\{110\}$  and  $\{112\}$  boundaries studied clearly showed that the ability of these boundaries to move under capillary driving force depends crucially on the initial boundary inclination. While boundaries with an initial inclination near  $\{112\}$  can easily assume a curved shape and therefore migrate, boundaries with an initial  $\{110\}$  plane remain flat or form non-mobile facets and therefore do not move. The reason for this behavior is apparently the substantial anisotropy of the inclination dependence of the energy  $\gamma(\psi)$  of  $60^\circ\langle 111 \rangle$  tilt boundaries with differently high torque  $d\gamma/d\psi$  around  $\{112\}$  and  $\{110\}$  inclinations, as revealed by atomistic simulations of the respective boundaries. Therefore, for  $\Sigma 3$   $60^\circ\langle 111 \rangle$  tilt boundaries there is no uniform tilt grain boundary mobility, as it was observed in the past for numerous (curvature driven) high angle grain boundaries in Al bicrystals.

The  $\Sigma 3$   $70.5^\circ\langle 110 \rangle$  tilt boundary with the geometry of the coherent  $\{111\}$  twin boundary and the boundaries with a deviation of the tilt angle up to  $6^\circ$  from  $70.5^\circ\langle 110 \rangle$  misorientation remained flat/straight in the experiments maintaining their initial inclinations. This is obviously due to the very low energy associated with the  $(111)$  boundary plane (coherent twin) and the high torque value around this inclination.

The  $59.2^\circ\langle 111 \rangle$  tilt grain boundary with a geometry very close to the  $\Sigma 3$   $\{110\}$  incoherent twin boundary, which did not migrate at all under the capillary driving force, was observed to be quite mobile under applied mechanical stress. However, in contrast to the results of numerous previous experiments with different grain boundaries in Al bicrystals, this boundary moved with a zero coupling factor, i.e. without producing any measurable shear parallel to the boundary plane.

The results of this work and their interpretation were published in Acta Materialia:


Jann-Erik Brandenburg, Luis A. Barrales-Mora, Sadahiro Tsurekawa, Dmitri A. Molodov:  
Dynamic behavior of grain boundaries with misorientations in the vicinity of  $\Sigma 3$  coherent and incoherent twin boundaries in Al bicrystals, Acta Materialia, 2023, v. 259, 119272.  
<https://doi.org/10.1016/j.actamat.2023.119272>.

(v) In the reference period, further important progress was achieved in the other part our joint research, namely the experimental and computational investigation of the effects of specific grain boundaries on the local mechanical properties in aluminum bicrystals. The nanoindentation measurements on Al bicrystals with  $\Sigma 3[110](\bar{1}11)$  and  $\Sigma 3[110](\bar{1}12)$  grain boundaries were successfully completed. The discussion of the obtained results and their comparison with the previously obtained data revealed the need to perform some additional experiments, for which bicrystal samples with a  $70.5^\circ\langle 110 \rangle$  tilt boundary with the geometry of the  $\Sigma 3$  coherent twin boundary are required. These samples are being prepared in Aachen and the measurements will be carried out over the next few months.

(vi) With a view to the future development of our research and the recruitment of potential coworkers for our projects, it is worth mentioning that, at my suggestion, one of the PhD students at the Institute of Physical Metallurgy and Materials Physics in Aachen, M.Sc. Maximilian Wollenweber, who is interested in a postdoctoral position after completing his PhD program, visited Kumamoto University in September 2023. In a conversation with Prof. Tsurekawa, he was informed about the current research projects in the laboratory and the possibilities of applying for the postdoctoral position at Kumamoto University under the corresponding IROAST program. He was also warmly welcomed by the students of Prof. Tsurekawa, who showed him around the laboratory facilities, Kumamoto University and the city of Kumamoto.



## FY2023 IROAST Research Activity Annual Report–Distinguished Professor

No.2-1-3	Nanoscale assemblies in hydrogen-bonded liquids and in amorphous materials			
Name	László PUSZTAI	Title	Scientific advisor	
Affiliation	HUN-REN Wigner Research Centre for Physics, Hungary Email: pusztai.laszlo@wigner.hun-ren.hu			
Research Field	Advanced materials / Data science			
Period of appointment	April 1, 2023- March 31, 2024			
Host Professor	Ichiro AKAI and Shinya HOSOKAWA			
Affiliation	Institute of Industrial Nanomaterials, KU Email: iakai@kumamoto-u.ac.jp shhosokawa@kumamoto-u.ac.jp	Title	Professor	

### 1. Research achievements

#### Symposiums/seminars for graduate students/undergraduate students in KU

I have delivered a 90-minute presentation as an *IROAST Seminar* (Kumamoto University, 7 November 2023), titled ‘*Understanding the structure of liquids: from the stone age to artificial intelligence*’.



#### Academic research papers published from 2023/4 to 2023/12 (under the name of IROAST)

Yamada H., Ohara K., Hiroi S., Sakuda A., Ikeda K., Ohkubo T., Nakada K., Tsukasaki H., Nakajima H., Temleitner L., **Pusztai L.**, Ariga S., Matsuo A., Ding J., Nakano T., Kimura T., Kobayashi R., Usuki T., Tahara S., Amezawa K., Tateyama Y., Mori S., Hayashi A.; Lithium Ion Transport Environment by Molecular Vibrations in Ion-Conducting Glasses; *ENERGY AND ENVIRONMENTAL MATERIALS* Paper: e12612, 10 p. (2023)



DOI: <https://doi.org/10.1002/eem2.12612>

Pethes, I.; **Pusztai, L.**; Temleitner, L.; Evolution of the hydrogen-bonded network in methanol-water mixtures upon cooling; *JOURNAL OF MOLECULAR LIQUIDS* 386 Paper: 122494, 13 p. (2023)

DOI: <https://doi.org/10.1016/j.molliq.2023.122494>

S. Hosokawa, J. R. Stellhorn, N. Boudet, N. Blanc, E. Magome, **L. Pusztai**, S. Kohara, K. Ikeda, and T. Otomo; Local- and intermediate-range partial structure study of As-Se glasses; *JOURNAL OF PHYSICAL OF JAPAN* 93 Paper: 014601, 12 p. (2024)

DOI: <https://doi.org/10.7566/JPSJ.93.014601>

\*Scheduled to be issued on January 15, 2024

### **Implementation and progress of international joint research**

My primary research goal in general may be described in short as ‘*understanding disordered structures*’. Accordingly, my main activity (still, in general) is the investigation of the microscopic structure of liquids, amorphous materials and disordered crystals. We combine experimental data, such as total scattering structure factors (TSSF) from X-ray and neutron diffraction (XRD and ND, respectively) and EXAFS spectra, with computer modeling tools, such as Reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations. As a result of such an approach, large sets (containing tens of thousands) of atomic coordinates (‘particle configurations’) in simulation boxes are provided that are consistent (within errors) with experimental data. These configurations are then subjected to various geometrical analyses, so that specific questions concerning the structure of a material may be answered. Below I describe some selected results from the fiscal year of 2023.

(i) *On the structure and dynamics of materials relevant for energy storage.* – Controlling Li ion transport in glasses at atomic and molecular levels is key to realizing all-solid-state batteries, a promising technology for electric vehicles. In this context,  $\text{Li}_3\text{PS}_4$  glass, a promising solid electrolyte candidate, exhibits dynamic coupling between the  $\text{Li}^+$  cation mobility and the  $\text{PS}_4^{3-}$  anion libration, which is commonly referred to as the paddlewheel effect. In addition, it exhibits a concerted cation diffusion effect (i.e., a cation–cation interaction), which is regarded as the essence of high Li-ion transport. However, the correlation between the  $\text{Li}^+$  ions within the glass structure can only be vaguely determined, due to the limited experimental information that can be obtained. Here, this study reports that the Li ions present in glasses can be classified by evaluating their valence oscillations via Bader analysis to topologically analyze the chemical bonds. It is found that three types of Li ions are present in  $\text{Li}_3\text{PS}_4$  glass, and that the more mobile Li ions (i.e., the Li3-type ions) exhibit a characteristic correlation at relatively long distances of 4.0 to 5.0 Å (0.4 to 0.5 nm). Furthermore, reverse Monte Carlo simulations combined with deep learning potentials, that reproduce X-ray, neutron, and electron diffraction pair distribution functions, showed an increase in terms of the number of Li3-type ions for partially crystallized glass structures with improved Li ion transport properties. Our results show order within the disorder of the Li ion distribution in the glass by a topological analysis of their valences. Thus, considering the molecular vibrations in the glass during the evaluation of the Li ion valences is expected to lead to the development of new solid electrolytes.

**Related publication:** Yamada H., Ohara K., Hiroi S., Sakuda A., Ikeda K., Ohkubo T., Nakada K., Tsukasaki H., Nakajima H., Temleitner L., **Pusztai L.**, Ariga S., Matsuo A., Ding J., Nakano T., Kimura T., Kobayashi R., Usuki T., Tahara S., Amezawa K., Tateyama Y., Mori S., Hayashi A.; Lithium Ion Transport Environment by Molecular Vibrations in Ion-Conducting Glasses; *ENERGY AND ENVIRONMENTAL MATERIALS* Paper: e12612, 10 p. (2023)

(ii) *The temperature-dependent structure of methanol-water liquid mixtures.* – The hydrogen-bonded structure of methanol – water mixtures have been investigated over the entire alcohol concentration range (from  $x_{\text{Methanol}} = 0.1$  to 1.0) at several temperatures, from 300 K down to the freezing point of the given mixture. Classical molecular dynamics simulations have been carried out, using the all-atom OPLS-AA force field for methanol and the TIP4P/2005 model for water molecules. Simulation trajectories ('particle configurations') have been analyzed, in order to characterize the hydrogen-bonded network in the mixtures. The temperature and concentration dependence of the average hydrogen bond (H-bond) numbers between different types of molecules, the donor/acceptor roles of water and methanol molecules, and hydrogen bond number distributions have been revealed. The topology of the total system, as well as that of the water and methanol subsystems, has been investigated by calculating the cluster size distributions, the number of primitive rings, and ring size and ring type distributions. It has been found that upon cooling, the average number of H-bonded water molecules increases at every concentration and temperature investigated. As far as the connectivity of the hydrogen-bonded network is concerned, the percolation threshold has been shown to be above  $x_M = 0.9$  already at room temperature.

**Related publication:** Pethes, I.; Puzsai, L.; Temleitner, L.; Evolution of the hydrogen-bonded network in methanol-water mixtures upon cooling; *JOURNAL OF MOLECULAR LIQUIDS* 386 Paper: 122494, 13 p. (2023)

## ***2. Prospect for further research collaboration with Kumamoto University***

During FY 2023, I've collaborated mostly with my host professor, Dr. Hosokawa, and Dr. Nakajima from FAST.

The joint research work with Dr. Nakajima, on high pressure diffraction measurements on various liquid mixtures, has evolved into a joint KAKENHI proposal with him, which proposal was approved in FY2022.

Follow-up publications with Prof. Hosokawa on the structure of amorphous materials will continue to appear for a while (at the moment, there is one publication accepted and scheduled to appear in 2024, as well as another one submitted).

## FY2023 IROAST Research Activity Annual Report–Distinguished Professor

No.2-1-4	Development and management of biomaterials			
Name	Yufeng ZHENG	Title	Professor	
Affiliation	School of Materials Science and Engineering, Peking University, China Email: yfzheng@pku.edu.cn yfzheng@kumamoto-u.ac.jp			
Research Field	Biotechnology & healthcare technology / Advanced materials			
Period of appointment	April 1, 2023- March 31, 2024			
Host Professor	Yoji MINE			
Affiliation	Faculty of Advanced Science and Technology Email: mine@msre.kumamoto-u.ac.jp	Title	Professor	

### Details of Activities

#### 1. Research achievements

The fiscal year 2023 report covers a two-day visit to Kumamoto University's IROAST from March 21 to 23. During the visit, I engaged in research discussions with Prof. Mine's laboratory on corrosion fatigue testing using small ring specimens. The study focused on Zn-Li biodegradable implant alloys with various compositions. At Kumamoto University, ring-shaped specimens will be prepared, and fatigue tests will be conducted in both atmospheric and simulated body environments to elucidate the effects of alloy additions on fatigue crack propagation and fatigue life. The results obtained will be reviewed during the next visit. Additionally, I visited Professor Lee's laboratory at IINa to exchange information on biomaterials.

The followings are academic research papers published from 2023/4 to 2024/3

Zhenning Su, Cancan Yao, Joanne Tipper, Lijun Yang, Xiangbo Xu, Xihua Chen, Guo Bao, Bin He\*, Xiaoxue Xu\*, and Yufeng Zheng,\* "Nanostrategy of Targeting at Embryonic Trophoblast Cells Using CuO Nanoparticles for Female Contraception," ACS Nano, 17, 24, 25185–25204 (2023)

Q Jia, Q. Jia, S. Zhu, Y. Zheng, Y. Mine, K. Takashima, S. Guan, „A promoting nitric oxide-releasing coating containing copper ion on ZE21B alloy for potential vascular stent application," Journal of Magnesium and Alloys, 11 (12), 4542-4561 (2023)

Li-Xin Long, Fen-Fen Chen, Lan-Yue Cui, Ze-Song Wei, Hai-Tao Wang, Rong-Chang Zeng, Yu-Feng Zheng, "Comparison of microstructure, mechanical property, and degradation rate of Mg-1Li-1Ca and Mg-4Li-1Ca alloys," Bioactive Materials 26, 29-291 (2023)

Wang, Shufang; Liu, Tingting; Nan, Nan; Lu, Cong; Liang, Min; Wang, Siyu; Wang, Hu; He, Bin; Chen, Xihua; Xu, Xiangbo; Zheng, Yufeng Exosomes from Human Umbilical Cord Mesenchymal Stem Cells Facilitates Injured Endometrial Restoring in Early Repair Period through miR-202-3p Mediating Formation of ECM  
Stem Cell Reviews and Reports, 19, 6, 1954-1964 (2023)

Xiehui Chen, Rong Chang, Hongtao Liu, Le Zhang, Yufeng Zheng, „Moving research direction in the field of metallic bioresorbable stents-A mini-review”, *Bioactive Materials* 24, 20-25(2023)

Zheng, Yufeng; Liu, Xiao; Shen, Danni; Li, Wenting; Cheng, Yan; Yang, Ming; Kou, Yuhui; Jiang, Baoguo, “Perceiving the connection between the bone healing process and biodegradation of biodegradable metal implants through precise bioadaptability principle,” *Journal of Materials Science & Technology* 147, 132-144 (2023)



## 2. Prospect for further research collaboration with Kumamoto University

This visit was short, lasting only two days, but it marked the first post-pandemic visit to IROAST. In the fiscal year 2024, I plan to conduct in-depth joint research with Professor Mine, host seminars for researchers and graduate students, and deliver lectures for undergraduate students.