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Exploring Diversified Teaching Methods in the Fundamentals of Materials Science and Engineering Course Guided by Computer Simulation

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Abstract:

Materials Science and Engineering is a fundamental course for materials-focused majors in higher education institutions, encompassing a broad spectrum of knowledge systems. Traditional teaching methods often struggle to achieve optimal results. To address this, we have implemented reforms in the theoretical course of Materials Science and Engineering, guided by computer simulation and aligned with the goals of fostering innovation and entrepreneurship. These reforms span teaching content, teaching methodology, assessment criteria, and the integration of research. Our findings reveal that incorporating computer simulation into classroom instruction not only effectively bridges scientific research resources with traditional teaching practices but also boosts students' engagement, enhances classroom efficiency, and ensures a comprehensive grasp of the fundamentals of materials science and engineering.

Keywords:

Materials science and engineering
Computer simulation
Innovation and entrepreneurship
Diversified teaching exploration

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1. Introduction

The Ministry of Education emphasized in the National Conference on Undergraduate Education in Higher Education Institutions the adherence to the principle of "focusing on undergraduates," promoting the "Four Returns," accelerating the construction of high-level undergraduate education, comprehensively improving talent cultivation capabilities, and nurturing a new generation capable of shouldering the great responsibility of national rejuvenation [1]. Carrying out innovation and entrepreneurship reforms in higher education classrooms is an effective measure to respond to the spirit of the National Conference on Undergraduate Education in Higher Education Institutions. Innovation and entrepreneurship education, referred to as double innovation education, is a practical education that deepens higher education reform and cultivates talents with entrepreneurial and innovative consciousness [2] and groundbreaking abilities [3]. The reform of double innovation education is a new concept for talent cultivation in universities [4] and an important measure to alleviate the employment pressure of college students and promote social and economic growth [5].

Integrating double innovation education into basic courses for engineering majors can not only achieve the course goal of applying learned knowledge but also enhance students' mastery of basic knowledge, cultivating innovative and composite talents with critical thinking, innovative consciousness, and entrepreneurial spirit [6]. This article takes the course Fundamentals of Materials Science and Engineering as an example to explore diversified teaching reforms by integrating elements of double innovation into basic courses for engineering majors in the context of innovation and entrepreneurship.

Fundamentals of Materials Science and Engineering is a theoretical and fundamental course that studies the commonalities of solid materials. It is also an important link in the talent cultivation system for materials science. This course focuses on explaining the interrelationships between material composition, structure, preparation processes, and properties [7]. However, this course covers a wide range of knowledge, and its content is abstract and conceptual, which makes it boring and difficult for most students to learn over the years. The traditional teacher-centered and indoctrination-style teaching method in the classroom has yielded very unsatisfactory results [8].

Recently, to encourage teachers to rely on teaching practices to carry out innovation and entrepreneurship education, this course has been included in the innovation and entrepreneurship curriculum of Nanchang Hangkong University. With the re-discussion and compilation of the course syllabus, there has been a contradiction between "increasing knowledge information and corresponding reductions in class hours," which has further increased the difficulty of teaching and learning in the classroom. In particular, it is difficult for students to understand the microscopic dynamic response laws of materials under specific conditions, as the traditional PowerPoint teaching mode cannot abstract specific dynamic images. How to find an effective carrier to simplify the difficulty of course understanding and stimulate students' interest in learning is the primary problem faced by the current course.

With the rapid development of computer technology and materials simulation theory, computational simulation has become an important means of teaching [9] and scientific research [10] in the frontier field of contemporary materials science. Exploring the teaching mode of deep integration of interdisciplinary subjects also provides important opportunities for innovation and entrepreneurship reforms in higher education in China. The reform focuses on how to use computer simulation as a carrier to effectively build and utilize computational resources to address the pain points and difficulties in traditional teaching. There are many simulation software in materials science research [11], including commercial software such as MATERIAL STUDIO, VASP, and ABAQUS, as well as open-source software such as VESTA, SIESTA, LAMMPS, and OVITO. Introducing these software into the Fundamentals of Materials Science and Engineering classroom can not only visually demonstrate the microscopic structure of crystals [12] and the microscopic dynamic response modes of materials under specific conditions but also mobilize the classroom atmosphere and improve classroom efficiency. This study takes students from the Composite Materials and Engineering major at Nanchang Hangkong University as the subject and summarizes the reform effectiveness and experience from four aspects: teaching content, teaching methods, assessment forms, and the integration of science and education. It provides reference significance for cultivating interdisciplinary innovative and entrepreneurial talents.

2. Exploration of teaching reform

2.1. Enrichment of teaching content

Considering the academic situation and course objectives, teachers identified the microscopic structure of crystalline materials and their response under specific conditions as a challenging aspect of the course. This is because it requires students to possess strong three-dimensional spatial imagination. Students majoring in Composite

Materials Engineering and Polymer Materials have not taken crystallography courses and thus lack three-dimensional spatial imagination. In previous classroom teaching, students generally found these chapters difficult. Based on this situation, there is currently a lack of effective cases that can deepen students' understanding of material structure and properties. To more intuitively demonstrate the microscopic structure and dynamic response laws of materials, material simulation cases from scientific research projects can be introduced into the classroom, thereby enriching teaching content and stimulating students' interest in learning.

The course teachers have many years of experience in material design and simulation and have presided over and participated in multiple national and provincial-level material design and simulation research projects. Making simulations from research projects into dynamic videos or series of pictures for classroom presentation and explanation can achieve twice the result with half the effort. In the course teaching, the knowledge points where computer simulation cases have been introduced are listed in **Table 1**. These cases partly come from the research projects of the course teachers and partly from simulations conducted in students' second classrooms. Combining these cases can explain the difficult points of the course more vividly.

For example, when explaining the crystal structure of metallic materials, the teacher demonstrates how similar atoms can have completely different lattice constants, elastic constants, thermal expansion coefficients, and other ground-state properties under different stacking modes through VASP calculations. This helps students deepen their understanding of the significant impact of crystal structure on material properties. When reviewing the applications of carbon materials, the compression of carbon nanotubes is demonstrated through OVITO, allowing students to clearly see the dynamic process of carbon nanotube collapse. When introducing crystal point defects, cases of metal material defect formation under neutron irradiation conditions are presented. Based on LAMMPS calculations, it is possible to clearly showcase vacancies, interstitial atoms, Frenkel defects, and Schottky defects in metal materials under neutron irradiation. When explaining knowledge points such as dislocation types, dislocation slip, and climb, a case of dislocation slip during interface stretching is introduced. The formation of slip systems, dislocation slip, and evolution laws can be visually demonstrated through the OVITO centrosymmetric parameter coloring method [9]. **Figure 1** clearly showcases some of the simulation cases introduced into the teaching content. These cases turn the microscopic into macroscopic in classroom demonstrations, simplifying the learning difficulty of the course. Their introduction into the curriculum not only enriches classroom teaching content, reveals the microscopic structure and intrinsic dynamic processes of materials, and stimulates students' interest in tracing the origins of material phenomena, but also cultivates material research and development talents with computational thinking, meeting the national demand for the development of computational theory and materials science.

2.2. Diversification of teaching methods

In the past, this course was primarily taught through a combination of blackboard writing and PowerPoint presentations, utilizing a unidirectional teaching approach that often led to students losing focus in the

Table 1. Knowledge points of computer simulation cases introduced in classroom teaching

Chapter	Knowledge points	Chapter	Knowledge points
Two	Interaction and Bonding between Atoms	Three	Unit Cell Structure and Properties of Alloy Materials
Two	Characteristics and Types of Crystals	Three	Unit Cell Structure and Properties of Inorganic Non-metallic Materials
Two	Point Defects in Crystals	Three	Microstructure and Properties of Polymer Materials
Two	Linear Defects in Crystals	Three	Microstructure and Properties of Composite Materials
Two	Diffusion Coefficient and Diffusion Path	Four	Deformation of Materials

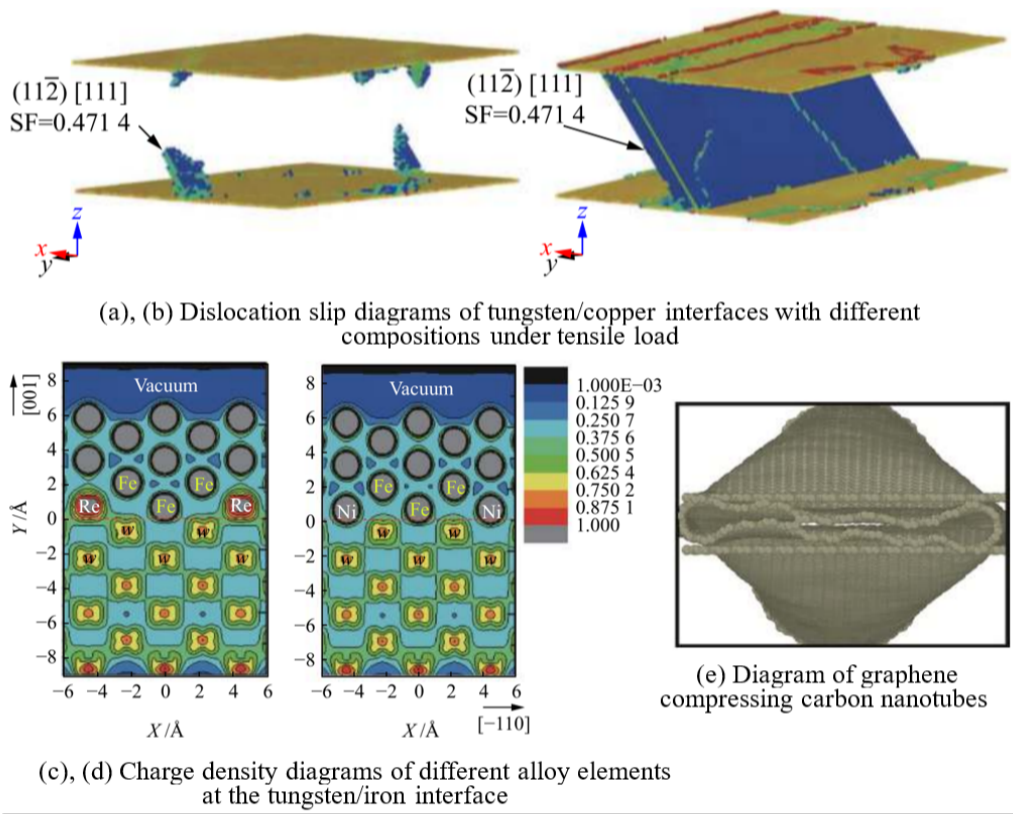

Figure 1. Schematic diagram of material simulation cases introduced into the teaching content

classroom. The introduction of simulation techniques can improve this situation, diversify teaching methods, and stimulate students' interest in learning. During the course, two additional teaching methods, interactive teaching and flipped classroom, have been implemented. Course instructors integrate simulations into the primary classroom, effectively simplifying complex course content and enabling flexible interactive teaching. For instance, when studying the stacking of atoms in crystals, most students struggle to understand the arrangement of atoms on close-packed planes in different crystal structures. By demonstrating the stacking process of crystal structures using VESTA software, abstract concepts are transformed into concrete visualizations, enabling students to gain an intuitive understanding. It is worth mentioning that material modeling and computational processes also pique students' interest and broaden their horizons, thereby facilitating their engagement in computational simulation practices in the secondary classroom.

The integration of simulation software, supercomputing resources, and the Chaoxing online teaching platform enables the implementation of the flipped classroom teaching method. Through careful design of both the first and second classrooms, difficult problems can be addressed in a flipped classroom setting [13]. This design process includes selecting students, identifying and posting difficult problems, and providing training on simulation workflows and computational software. Initially, computational tasks are posted on the online platform, and simulation workflows are established to attract student participation. Utilizing supercomputing resources, students engage in simulation training for difficult problems in the second classroom. The theories underlying these simulations, the simulation processes themselves, and the conclusions drawn from them become key content for student presentations in the flipped classroom. Subsequently, in the first classroom teaching session, the focus is on classroom activities centered around the simulation results presented by some students. This approach stimulates critical thinking among a larger group of students, fostering a lively discussion-based learning environment. The teacher emphasizes innovative thinking and understanding of key concepts, providing feedback and supplementary explanations to address any errors or gaps in the student presentations, thereby effectively extending the learning beyond the classroom. The flipped classroom approach transforms the traditionally dull classroom atmosphere, promoting a deeper understanding of knowledge points and cultivating students' enthusiasm for independent learning. It is worth noting that due to time constraints, the flipped classroom sessions are limited to 2–6 hours. Practical experience has demonstrated that introducing simulation tools into the Fundamentals of Materials Science and Engineering course enhances students' independent learning, computational thinking, and material development capabilities. This approach effectively bridges the gap between multiple disciplines in the new educational landscape. The combination of theoretical explanations in the first classroom and practical applications in the second classroom significantly improves the quality of course instruction and talent cultivation.

2.3. Innovation in assessment methods

Previously, the assessment of this course mainly consisted of two parts: regular performance and exam scores. Regular performance accounted for 30%, while exam scores accounted for 70%. Teachers mainly assigned regular scores based on students' classroom attendance, classroom participation in answering questions, and after-class assignments. However, this assessment method was relatively simplistic, resulting in minimal differences in regular scores among students over the years. Consequently, the final assessment score was primarily determined by the exam score. The introduction of simulation content into the assessment can improve the scoring method for regular performance. Specifically, regular performance is divided into 10% for simulation tasks and 20% for classroom performance. Simulation tasks are designed for knowledge points that students find difficult and abstract. These tasks, along with their requirements, are published on the Chaoxing online teaching platform. In the second classroom, students freely form groups and select a set of simulation tasks to complete. For these tasks, students can communicate with teachers on the online platform, WeChat, or QQ groups. Through simulation, students can understand abstract problems and grasp difficult knowledge. During the assessment, teachers ask questions about key concepts and difficult issues related to the simulation tasks, and students provide answers. Teachers then assign scores based on students' responses. To stimulate students' interest, they have the option to present their simulation tasks in a flipped classroom, which would earn them a full score for that component. This enhanced assessment method not only encourages students to participate in second classroom simulation tasks and understand key and difficult concepts but also provides a more substantial basis for scoring regular performance. It offers opportunities for teachers and students to discuss issues, improves teachers' role identification among students, and achieves the goal of mutual progress.

2.4. Integration of teaching and scientific research

With the technological revolution and significant economic and social changes, university teachers are required to juggle teaching, scientific research, and educating students. The current trend in higher education is to achieve the integration of teaching and scientific research outcomes and cultivate innovative and entrepreneurial talents who meet the needs of society. By combining course teaching objectives with scientific research projects, course teachers can cultivate students' interest and guide them to actively participate in scientific research tasks through open and shared computing resources, designing and decomposing research projects, and developing a series of assessment methods. With careful selection and reasonable design, the decomposed tasks for simulation are moderately challenging for students. Discussing and solving these tasks not only deepens students' understanding of key and difficult concepts but also promotes independent learning through scientific research. The insights and challenges encountered during these simulation tasks can serve as important material for student presentations in flipped classrooms and teachers' assessment and feedback on regular performance. This integrated approach to teaching and scientific research will stimulate teaching vitality and boost students' innovation and entrepreneurship capabilities in a multidisciplinary context.

3. Effectiveness of teaching reform

After collating the teaching feedback and evaluation of the Fundamentals of Materials Science and Engineering course from 2017 to 2019, this article summarizes the typical issues raised as presented in **Figure 2**. Through an analysis of **Figure 2**, it can be seen that most students believe the Fundamentals of Materials Science and Engineering course is moderately difficult after the reform. By introducing simulated cases into the teaching content, most students can deepen their understanding of concepts through the presentation of these cases, effectively simplifying the difficult points of the course. Through the introduction of research tasks into the assessment, most students can complete hands-on activities, which have honed their practical skills and promoted their self-learning abilities. Finally, as evident from the figure, the implementation of teaching reforms has increased most students' interest in the course. However, it cannot be ignored that there are also shortcomings in the reform, particularly regarding participation in research tasks. Since the assessment is conducted in a group format, there are still many students (about 21%) who are not actively engaged. In this regard, the course applicant intends to increase the proportion of student presentations in the assessment for the upcoming course teaching, offer open experiments, encourage less-engaged students to participate, and conduct more one-on-one discussions with students during the teaching process. These measures are aimed at guiding less-engaged students to be more invested in the theoretical learning and practical research tasks of the course, thereby improving their participation.

Through recent years of course teaching reforms and experience accumulation, the introduction of computer simulation into the Fundamentals of Materials Science and Engineering course has achieved certain results. The reform has significantly improved students' self-learning abilities and initiative, and noticeably enhanced interactive teaching in the primary classroom. Through the decomposition and implementation of research tasks, students' hands-on research skills in the secondary classroom have also gradually improved, and their interest in learning has increased year by year. In

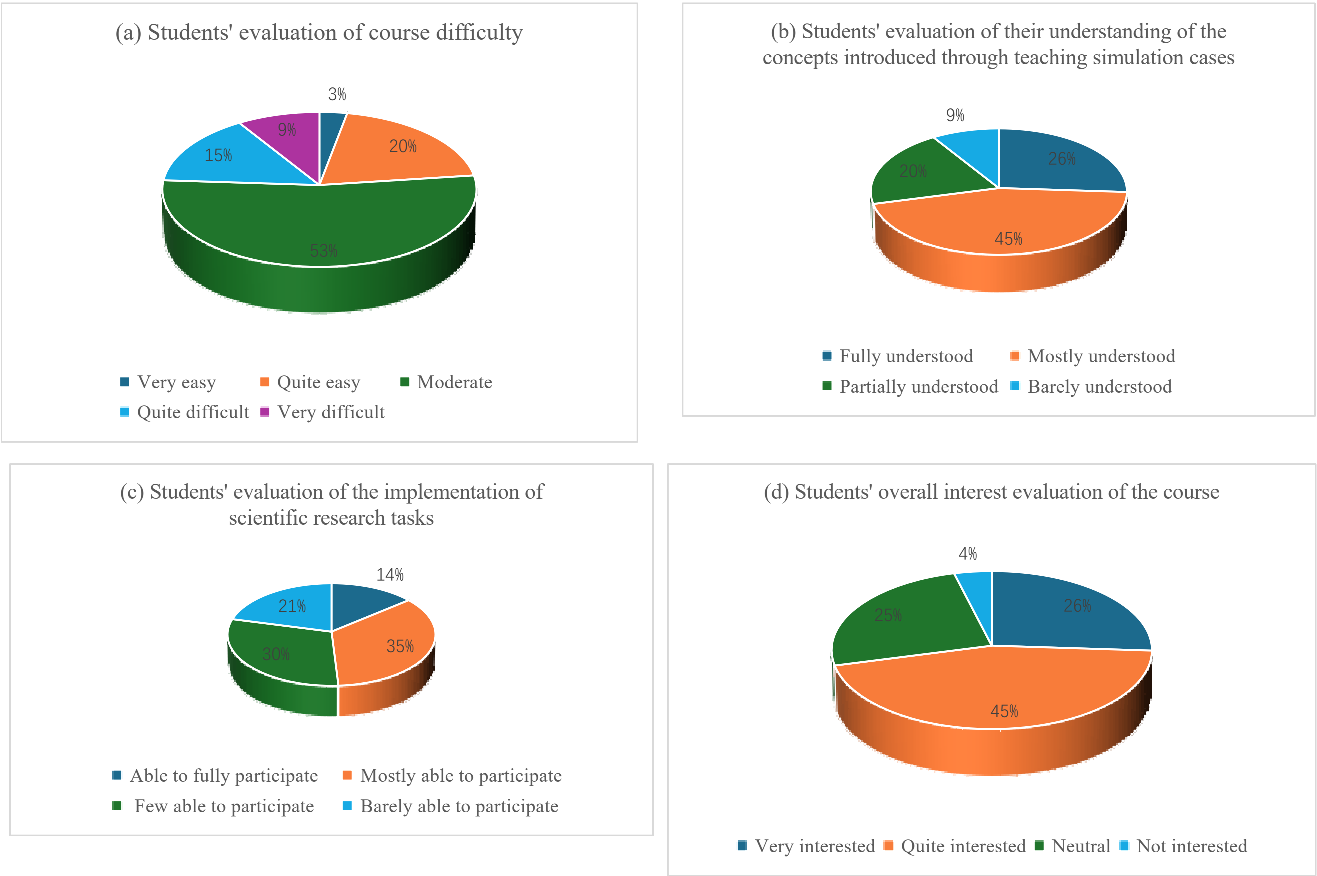

Figure 2. Graphical analysis of typical student feedback data from 2017–2019

the comparison of student performance from 2017 to 2019, the proportion of students failing the course has decreased annually. Student evaluations of teaching have risen year after year, and student satisfaction with the course has also increased significantly. In response to the current teaching reform goal of integrating innovation and entrepreneurship elements into basic engineering courses to stimulate students' self-learning enthusiasm, this article greatly enriches the teaching content through the introduction of computer simulation methods, achieving diversified reforms in teaching methods and assessments. Ultimately, this approach has stimulated students' autonomy in learning, simplified the difficulty of the course, promoted cross-integration between related disciplines, and provided a reference for cultivating materials professionals with computational thinking.

4. Conclusion

In the context of multidisciplinary integration, the development of teaching methods and philosophies in higher education has become diversified and comprehensive. The rapid advancement of theoretical computation provides a significant opportunity for reforming innovation and entrepreneurship education in China. This article introduces computer simulation as a vehicle for teaching reform in the Fundamentals of Materials Science and Engineering course in the primary classroom. The aim of this curriculum reform is to enhance classroom effectiveness, expand course content, explore the integration of science and education, and cultivate innovative and entrepreneurial talents who are capable of assuming the responsibility of national rejuvenation. Through the implementation of teaching reforms, not only has the classroom atmosphere improved and teaching effectiveness enhanced, but students' interest and initiative in learning have also increased. Additionally, students' innovation and entrepreneurship abilities as well as their sense of teamwork and collaboration have been honed. Simultaneously, with the progression of the reforms, teachers' role recognition among students has gradually improved. These effective reform experiences can provide some references and guidance for other curriculum reforms in materials-related majors.

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Disclosure statement

The authors declare no conflict of interest.

References

[1] Ministry of Education, 2018, Declaration on First-Class Undergraduate Education ("Chengdu Declaration"). China University Teaching, 6: 4–5.

[2] Xie F, Wu L, 2020, Rethinking Entrepreneurship Education in Universities. Jiangsu Higher Education, 4: 91–95.

[3] Liang H, Xiong L, Zhou J, et al., 2019, Teaching Reform and Exploration of Polymer Physics Course under the Background of Innovation and Entrepreneurship. Journal of Nanchang Hangkong University (Natural Science Edition), 33(1): 112–116.

[4] Hou Y, Lin W, 2015, The Internal Coupling and Implementation Path of Entrepreneurship Education and the Transformation of Local Undergraduate Colleges. Higher Education Exploration, 2: 40–44.

[5] Gielnik MM, Frese M, Kahara-Kawuki A, et al., 2015, Action and Action-Regulation in Entrepreneurship: Evaluating a Student Training for Promoting Entrepreneurship. Academy of Management Learning and Education, 14(1): 69–94.

[6] Qin J, Li H, Chen X, 2020, Research on the Integration Strategy of New Engineering and Innovation and Entrepreneurship Education in Western Universities. Journal of Chongqing University of Arts and Sciences, 39(2): 119–132.

[7] Li Y, Zhai H, 2018, Research and Practice on the Teaching Model Reform of “Fundamentals of Materials Science” in Small Classes. North China Institute of Aerospace Engineering, 28(5): 45–47.

[8] Fu X, 2017, Exploring Effective Teaching Methods for Fundamentals of Materials Science. China Metallurgical Education, 183(6): 8–9.

[9] Zhang X, Tang D, 2019, Model Innovation of Information Technology-Assisted Teaching Activities. China University Teaching, 12: 54–60.

[10] Wei W, Chen L, Gong HR, et al., 2019, Strain-Stress Relationship and Dislocation Evolution of W-Cu Bilayers from a Constructed n-body W-Cu Potential. Journal of Physics: Condensed Matter, 31: 305002.

[11] Yang J, Fan Q, Yin S, 2015, Application of Diamond Software in the Teaching of “Fundamentals of Materials Science.” Journal of Leshan Normal University, 30(4): 108–110.

[12] Wen G, Bao X, Chen Y, et al., 2013, Application of Professional Software in the Teaching of “Fundamentals of Materials Science.” Journal of Suzhou University, 28(10): 89–93.

[13] Li G, Liu Y, Wang L, 2018, Role Orientation and Classroom Innovation of University Teachers under the Flipped Classroom Teaching Model. China University Teaching, 5: 69–72.

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