In honour of Professor Klaus Heinz

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PREFACE

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This issue is dedicated to Professor Klaus Heinz on the occasion of his 65th birthday. It contains original work by colleagues, who have enjoyed the privilege of collaborating with him and who wish to express their thanks and appreciation with selected contributions from their research.

In the scientific community the name Klaus Heinz will forever be associated with the method of low-energy electron diffraction (LEED). He dedicated the central part of his scientific work to the continuous and systematic advancement of this method and its application to ever new systems and to general questions of structural analysis. In the following, we will attempt to honour his scientific achievements and the personality behind the work.

Klaus Heinz studied physics in Mainz and after his diploma in 1968 he went to Fritz Stöckmann at the University in Karlsruhe to earn a doctorate in the field of experimental semiconductor physics in 1972 [1]. While leader of the research group *Photoleitung und elektrische Instabilitäten* in Karlsruhe, Klaus Heinz met Klaus Müller who had only recently returned from the USA. He was thus exposed to surface science, a subject then still in its fledgling stages, and especially to the method of low-energy electron diffraction that Klaus Müller had brought to Europe. This meeting would prove decisive for his future path in life. No doubt it was both the fascinating chance to venture into uncharted scientific terrain as well as the enthusiasm and charisma of Klaus Müller which induced him to accompany Klaus Müller to his newly founded *Lehrstuhl für Festkörperphysik* in Erlangen in 1973. In the beginning, it was not easy for the native of Palatine to adapt to the quite different Franconia. In the course of the years though, Franconia became—not only scientifically—a second home. As Klaus Heinz puts it *'man weint über Erlangen zweimal, einmal wenn man kommt und einmal wenn man geht!'*[1]. Well, he has not left and he was appointed associate professor at the *'Lehrstuhl für Festkörperphysik'*, in 1980. The following years saw him prefer Erlangen over external offers.

The close collaboration with Klaus Müller turned out to be exceedingly fruitful over the years, which was not least due to the two scientists complementing one another in their fundamental characteristics and thought patterns. On the one hand Klaus Müller, fiercely impulsive and with deep roots in experimentally oriented laboratory and development work and on the other hand level-headed Klaus Heinz, for whom understanding physics is the ability to express something formally correct by means of theoretical physics. His close proximity to theory, which Klaus Heinz retained during his entire scientific life, soon led him to delve into the interpretation of diffraction intensities, which are dominated by multiple scattering. His habilitation thesis, which he completed in 1977 in Erlangen, was dedicated to this topic [2]. Based on the algorithm for numerical calculation of these intensities, a problem solved by John Pendry only a few years before [3], Klaus Heinz began to research the implications for real systems. Initially he was occupied with the influence of experimental parameters on the structure of the spectra as well as the classification and relevance of individual scattering processes. These activities aimed to further develop efficient approximation procedures, that would allow, with the limited computational power of the seventies and eighties, to solve more than the simplest structures.

[1] 'You weep over Erlangen twice—once when you arrive and once when you leave!'

In a promising first approach, Klaus Heinz could show that the quasidynamical approximation, which neglects multiple scattering within the individual layers, delivers reliable results under certain experimental conditions, and with drastically reduced computing time [4].

The second outstanding figure that would significantly influence Klaus Heinz' scientific career was John Pendry (already cited above), with whom he spent his first sabbatical in the summer of 1985, to work with him on an extension of the LEED structure analysis on disordered adsorbate systems (diffuse LEED) [5]. This visit was the beginning of a highly successful collaboration that has continued for more than a decade and a close friendship that lasts to this day. Within the scope of this collaboration a number of essential steps were developed and tested, which turned the LEED structure analysis into the powerful and effective method it is today. Klaus Heinz was directly involved in these developments from the very beginning. It was always experiments in Erlangen that proved the capability of new concepts and over the years the theoretical and numerical work also relocated more and more to Erlangen. No doubt Pendry's idea to treat geometric deviations from a full dynamically calculated reference structure in a perturbative approach (tensor-LEED) [6] triggered this tempestuous development phase. This approach provided the final breakthrough for the LEED structure analysis—after all, it reduced the computing time necessary for a structure determination by several orders of magnitude. A few years later, Klaus Heinz and co-workers expanded this method to deal with chemical [7] and thermal [8] parameters. In combination with a highly efficient and automated parameter search algorithm [9] a programme package (`TensEr-LEED` code) was eventually made available to the public [10] and is today employed in many laboratories worldwide.

A number of ambitious approaches flowed from the collaboration with John Pendry and later with Pendry's former student Dilano Saldin. These went far beyond the conventional concept of *'trial-and-error'* structure analysis and permitted inference of surface structure directly from the measured intensities. The inversion of the tensor-LEED concept constituted a first approach, which allowed for a determination of the true structure directly from the difference between experimental and calculated intensities, provided a realistic reference model was chosen [11]. A considerably more far-reaching approach that was developed later is the holographic interpretation of the diffraction intensities, in which single prominent adatoms serve as beam splitters. This concept, initially formulated for disordered adatoms [12], was later expanded to ordered phases [13]. The development of LEED holography, recently mainly advanced by Dilano Saldin, promises an application to arbitrary surface structures [14]. This could signify a milestone in structural analysis, provided the problem of interfering contributions from multiple scattering can be reliably eliminated.

As impressive as his contributions to theoretical advancements of LEED structural analysis were, for the experimental physicist, Klaus Heinz, the application of these concepts on real systems always took centre stage. Hardly a class of systems exists whose surface crystallographic characterization he did not contribute to over the years with a number of excellent structure analyses. Thus his work comprises surface structure analyses of metals, semiconductors and even (doped) insulators. It spans from simple, clean surfaces via complex reconstructed phases to atomic and molecular adsorbate systems and epitaxial films. The statistics of the last version of *'NIST Surface Structure Database'* [15] (2003) found him in first place in international comparison with remarkably 138 solved surface structures, and in the following years he set this benchmark even higher. He was never concerned with the quantity of analyses his work group performed, it was rather the quality which ranked first, both from numerical and experimental quarters. Thus Klaus Heinz firmly established his Erlangen group at a world-class

level. Wherever structural information with crystallographic precision is required, he is sought after as collaborator, a fact well-documented by joint publications with more than 30 external groups.

Despite the variety of investigated systems, Klaus Heinz never settled for knowledge of the structure alone. True to his motto *'es gibt immer ein tieferes Verständnis'*[2], he always strove for theoretical confirmation and explanation of structures found in experiment. He constantly sought collaborations with other groups and never shrank from introducing new theoretical procedures in his own group. The eighties already saw him engaged in Monte Carlo simulations, to quantitatively determine the stability of adsorbate phases found experimentally [16]. For some time now he has trusted the supportive information from density functional theory, as it could quickly be shown that this method complements LEED structure analysis splendidly [17]. For similar reasons he introduced scanning-tunnelling microscopy in Erlangen, a tool long since indispensable to the investigation of epitaxial films, as experimental supplement to electron diffraction [18]. All in all the scientific work of Klaus Heinz currently encompasses close to 300 publications in reputable refereed journals as well as several chapters in edited books.

By virtue of his excellent scientific reputation and his integrity, Klaus Heinz was appointed to a number of national and international scientific committees. He organised several international conferences and was chairman of the surface science division and member of the Vorstandsrat of the Deutsche Physikalische Gesellschaft, as well as section editor for *Journal of Physics: Condensed Matter*. With the same commitment and sense of duty he worked as professor in Erlangen in academic self-administration and especially in teaching. He inspired generations of students with his well structured lectures that were characterized by a deep scientific understanding.

Klaus Heinz is not only esteemed as an excellent researcher and teacher, but also as an extraordinary person and outstanding figure. His personality is marked by absolute reliability and integrity. We particularly cherish his truly philanthropic outlook on life, from which stems that even during the fiercest controversy *'grundsätzlich der Mensch dahinter stehen bleiben muss'* [3]. These admirable character traits are paired with a keen sense of professional virtue and, beyond that, also personal problems and hardships of his students and co-workers, which Klaus Heinz meets with warm sympathy and selfless support. This is never directly restricted to only associates, but he rather endeavours to affect his whole environment similarly. It is certainly not without reason that generations of doctoral students at the *Lehrstuhl für Festkörperphysik* respectfully, and thus never in his presence, call him *'der Babba'* [4]. We wholeheartedly second this honorary title out of deep respect and sincere friendship.

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[2] 'There is always room for deeper scientific understanding'
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