1

Classical Theory and Atomistics

Many research workers have pursued the friction law. Behind the fruitful achievements, we found enormous amounts of efforts by workers in every kind of research field. Friction research has crossed more than 500 years from its beginning to establish the law of friction, and the long story of the scientific history of friction research is introduced here.

1.1 Law of Friction

Coulomb's friction law[1] was established at the end of the eighteenth century [1]. Before that, from the end of the seventeenth century to the middle of the eighteenth century, the basis or groundwork for research had already been done by Guillaume Amontons[2] [2]. The very first results in the science of friction were found in the notes and experimental sketches of Leonardo da Vinci.[3] In his experimental notes in 1508 [3], da Vinci evaluated the effects of surface roughness on the friction force for stone and wood, and, for the first time, presented the concept of a coefficient of friction.

Coulomb's friction law is simple and sensible, and we can readily obtain it through modern experimentation. This law is easily verified with current experimental techniques, but during the Renaissance era in Italy, it was not easy to carry out experiments with sufficient accuracy to clearly demonstrate the universality of the friction law. For that reason, 300 years of history passed after the beginning of the Italian Renaissance in the fifteenth century before the friction law was established as Coulomb's law.

The progress of industrialization in England between 1750 and 1850, which was later called the Industrial Revolution, brought about a major change in the production activities of human beings in Western society and later on a global scale. Research and development of machines necessary for various manufacturing industries was promoted. Improvement in the performance of lubrication technology was required together with machine design technology and machine processing technology.

1 Charles Augustin de Coulomb, 1736–1806, France.
2 Guillaume Amontons, 1633–1705, France.
3 Leonardo da Vinci, 1452–1519, Italy.

Friction at the Atomic Level: Atomistic Approaches in Tribology, First Edition. Motohisa Hirano.
© 2018 Wiley-VCH Verlag GmbH & Co. KGaA. Published 2018 by Wiley-VCH Verlag GmbH & Co. KGaA.

COPYRIGHTED MATERIAL

The laws of friction can be described as the following empirical laws.

1. The friction force is proportional to the force acting in the direction perpendicular to the surface of friction regardless of the apparent area of contact.
2. The dynamic friction force is independent of the speed of sliding motion.
3. The static friction force is greater than the dynamic friction force.

We can see friction at work in the various mechanical phenomena that surround us, and Coulomb's law can explain most of the nature of the dry friction of solid objects. For mechanical technology that supports industry, it goes without saying that friction is an important problem to be overcome. In the study of mechanical engineering, mechanical design that takes friction and contact phenomena into account ensures the efficiency of machinery. That fact made a detailed understanding of the nature of friction essential and motivated the research for the laws of friction.

Leonardo da Vinci conceived of friction experiments out of his own interest in science and interest in the shipbuilding technology of his day. His experimental records pointed to the material of the objects and surface roughness as factors that affect friction. Those experimental results founded the conjecture that friction is caused by mechanical locking of roughness on the surfaces of the objects. da Vinci also discovered that the friction force of dry solids is proportional to the weight of the object, which is perpendicular to friction force, and is independent of the area of contact far before the establishment of Coulomb's law. That proportionality of friction force and weight is linked to coming up with the concept of a coefficient of friction [4]. da Vinci also considered the difference between sliding friction and rolling friction. He thus revealed facts and laws that were entirely unknown before his research. After his work, the research on the origin of the appearance of friction had to wait for the appearance of an understanding based on atomistic theory and nanotechnology [5] for experimenting at the atomic level. Thus, for the next 200 years, the study of friction did not take the center stage in scientific research. The history of tribology and its related topics are shown in Figure 1.1.

The friction laws were established in the seventeenth and eighteenth centuries in France. At that time, shipbuilding, flower milling, and other industries thrived, and advances in mechanical design made the study of friction and mechanical components such as gears and bearings essential. On the foundation of advanced experimental techniques, the study of friction moved forward from the work of Amontons, Coulomb, and others, resulting in a deeper understanding of the nature of friction and the laws that describe it.

Amontons explained the lawful behavior of friction and the friction laws suggested by da Vinci through meticulous experimentation in 1699, proceeding with research to clarify why the friction laws hold by determining the causes [2]. Among the issues that Amontons tackled was the difficult problem of clarifying whether friction force is proportional to contact area. The common sense of the time was that friction force is proportional to the area of contact. In fact, there were experimental results that the friction force is proportional to the contact surface area when the surface is coated with a film of oil or other lubricant.

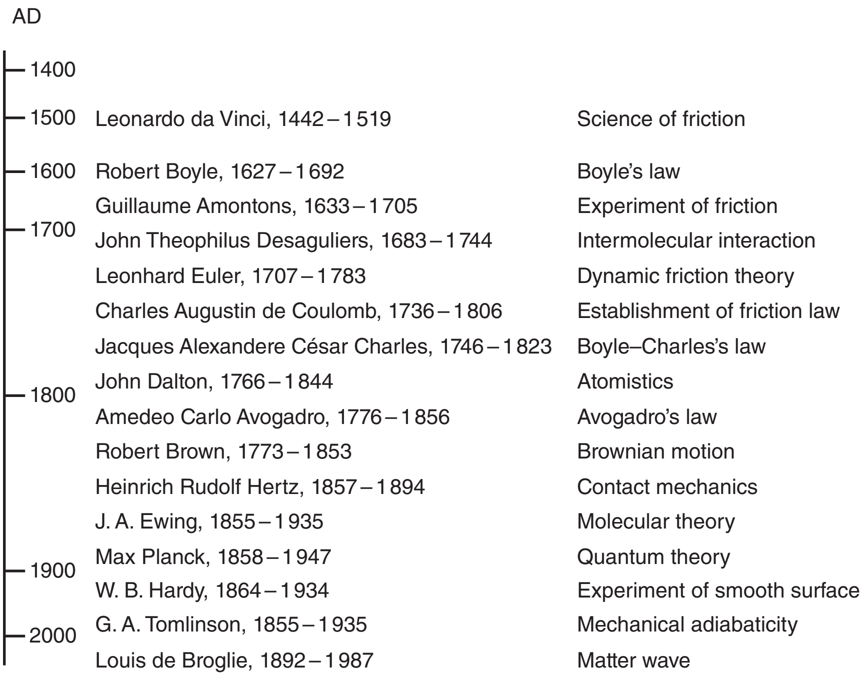

Figure 1.1 History of tribology.

Philippe de la Hire,[4] who lived in the same generation as Amontons, approached that problem with precise experimentation and showed that the friction force is proportional only to weight and is unrelated to the contact surface area in 1706 [6].

As the mechanics of Isaac Newton[5] was being systematized in the seventeenth and eighteenth centuries [7], there were attempts to incorporate friction force into the dynamics. At that time, friction force was a new force that was not dealt with in dynamics. Antonie Parent[6] solved the problem of an object taking friction force into account as a static equilibrium problem and published a paper in 1704 describing the concepts of the friction angle and friction cone [4]. Using Newton's mechanics as the foundation, Leonhard Euler[7] solved the problem of the sliding motion of an object with friction and provided the first theoretical basis in dynamics for the static friction coefficient being larger than the dynamic friction coefficient. The fact that the friction during sliding is often smaller than static friction could be explained by assuming that the asperities on one surface could jump part of the way over the gap between asperities on the other [8]. Euler solved the problem of belts and ropes wrapped around a cylinder as a dynamics

4 Philippe de la Hire, 1640–1718, France.
5 Isaac Newton, 1642–1727, United Kingdom.
6 Antonie Parent, 1666–1716, France.
7 Leonhard Euler, 1707–1783, Switzerland.

problem, showing that very large force is necessary for slippage of wrapped belts or ropes [4].

Charles Augustin de Coulomb was born in Angouleme, France in 1736. He made contributions of particular note in the fields of electromagnetism and mechanics [1]. In electromagnetics, he is well known for deriving the law of static electrical force. In the fields of physics and mechanical engineering, too, he is known for his great achievement in establishing the Coulomb's law of friction. The eighteenth century in France was an era in which culture, economics, and industry reached full maturity. There were strong gains in machine performance and durability, and overcoming friction was a major obstacle for those achievements. Before Coulomb, there were limits to the conditions that could be set in laboratory experiments, but advancement in the rapidly developing mechanical technology made it possible to obtain highly reliable practical data from actual machines. The French Academy of Sciences offered an award for excellent, highly practical research on friction. To meet the expectations, Coulomb submitted excellent research results for various types of friction, including flat surface friction, rope friction, pivot bearing friction, and rolling friction. Coulomb accurately solved the problem of flat surface friction and compiled dry friction experiments and theory to demonstrate the principles behind the friction law.

1.2 The Origin of Friction

The Japanese scientist Norimune Sota[8] wrote an interesting article on the scientific history of friction research [4]. The science of friction started in Italy during the Renaissance period in the fifteenth century. Leonardo da Vinci carefully observed and experimented on stones and wood found in daily life and introduced the concept of the ***friction coefficient***. More than 200 years passed without any progress in friction research, until much discussion of the laws regarding friction and the origin of friction started to happen in the seventeenth to eighteenth centuries. The results of research were applied to engineering in the form of lubrication technology during the Industrial Revolution in the eighteenth century, and research by Coulomb and others were summarized as laws of friction.

The principles of how friction happens at contacting surfaces were discussed from the end of the seventeenth century to around the middle of the eighteenth century as mentioned, and Coulomb completed his ***surface-roughness model***. Although surface roughness still sometimes could be an explanation of frictional behavior, the surface-roughness model basically fails to explain energy dissipation because of the gravitational force being the conservative force, as pointed out by John Leslie[9] in 1804 [9].

In contrast, John Theophilus Desaguliers[10] was aware of the importance of intermolecular force [10]. His idea, which is the root of the ***molecular theory***, is the complete opposite of the popular roughness theory, around the middle

8 Norimune Sota, 1911–1995, Japan.
9 John Leslie, 1766–1832, United Kingdom.
10 John Theophilus Desaguliers, 1683–1744, United Kingdom.

of the eighteenth century. After Desaguliers, during the 100 years until the nineteenth century, only one British physicist Samuel Vince[11] committed to Desaguliers' idea. The molecular theory considers the atomistic origin of friction to be the interaction of molecular forces at the surfaces where friction appears, as pointed out by James Alfred Ewing[12] in 1877 [11]. Accordingly, this theory claims that a smoother surface means that the friction surfaces come together, increasing the interference between surface forces. Desaguliers extracted a few millimeter-sized pieces from a lead sphere, and found in 1725 that strongly pressing such pieces against each other resulted in strong bonding between the pieces [10]. Further observation of the remains after separation showed that only a fraction of the pressed surface had actually been in contact. This finding in 1725 gave rise to the prediction that "*friction ultimately increases if surfaces are fully polished to very flat*." This prediction was proved by William Bate Hardy[13] in 1919 with improvements in surface processing technologies [12]. He is also well known as the first person to use the term ***boundary lubrication***. He carried out experiments on the friction of glass surfaces and showed that glass surfaces that are polished very carefully such as those in lenses have greater friction than glass with rough surfaces. He also found that tracks of wear caused by friction are initially about 1 μm wide, and as friction gradually increases wear, the width increases to about 50 μm. This experiment refuted the roughness theory and proved that friction is not only a problem of energy loss from the interaction of molecular forces but also is a phenomenon in materials science that accompanies fracture of the surface. The experiment done by Ragnar Holm[14] in 1936 demonstrated that the friction between clean surfaces is high under high vacuum and that minute amounts of gas molecule adsorption significantly decrease friction [13]. The modern ultrahigh-vacuum experiment of clean metal surfaces by Buckley showed a correlation with electronic properties such as the number of d-electrons [14]. Strang's experiment [15] done in 1949 proved that measured up-and-down motion of a solid in sliding was very small, and the corresponding work for the up-and-down motion was only 3–7% of the total work consumed by friction. These results showed the work for up-and-down motion stemming from the surface roughness was negligible. Thus, molecular theory gained evidence and became the foundation of the atomistics of friction.

On the other hand, regarding the friction model of actual surfaces, the contact model was refined through the concept of ***real area of contact*** proposed by Holm and Mises's material yield theory in plastic deformation [16]. Relations between friction forces and materials properties such as plasticity were investigated in detail in terms of ***adhesion theory*** based on shear models at the truly contacting and adhesive element [17–20]. A pair of contact asperities can be approximated as two spheres making elastic contact, that is, ***Hertzian contact*** by Hertz by[15] [21]. The findings resulted in today's lubrication technologies for head-disk interfaces in contact start-stop-type magnetic information storage disk

11 Samuel Vince, 1749–1821, United Kingdom.
12 James Alfred Ewing, 1855–1935, United Kingdom.
13 William Bate Hardy, 1864–1934, United Kingdom.
14 Ragnar Holm, 1879–1970, Germany.
15 Heinrich Rudolf Hertz, 1857–1894, Germany.

devices, and lubrication technologies on the small scale [22] will become even more important in miniature precision devices in the future.

1.3 Atomistics in Tribology

The work done by friction has a very different nature from the work done by gravity [4]. Work by gravity happens when objects are moved against gravity, which is always acting on objects. In contrast, friction is the force required to slide objects perpendicular to the direction of gravity. Once sliding motion starts, friction appears as resistance against the sliding motion and results in work by friction. Therefore, friction has the interesting property that it appears when objects start sliding and disappears when objects stop. Even in interatomic forces, no work by friction is generated as long as the combined interatomic force is perpendicular to the sliding direction. Leslie did not agree with Desaguliers' atomistic idea. Ewing stated in 1877, as mentioned, that friction force stems from molecular interaction at contacting surfaces. The British physicist Tomlinson [23] was the first to explain the energy dissipation stemming from molecular interaction at the start of the twentieth century, in 1929. He should have been inspired by the modern atomistics established by the British chemist John Dalton.[16]

Modern atomistics was established after physics reached the level of atoms in the nineteenth century. Physics started to consider atoms around the mid-nineteenth century, although the original concept of atomistics itself, which is that matter consists of atoms, is thought to have emerged in ancient Greece as ***particle philosophy***. The British physicist–chemist Robert Boyle[17] tried to use particle philosophy as the foundation of chemistry, and his attempt to build chemistry upon particle philosophy materialized in the early nineteenth century as Dalton's atomistics. Dalton postulated that objects with sizes that are touched daily, regardless of whether the objects are in gas, liquid, or solid state, consist of a vast number of very minute particles or atoms bound together by force. He thought that there is attraction and repulsion between atoms and that the balance between these opposing forces results in the three states of gas, liquid, and solid. The attraction and repulsion between atoms was later explained on the basis of the concept of electron energy levels and electron states in quantum mechanics. Dalton's atomistics was improved through corrections by Amedeo Carlo Avogadro[18] and others. Although there were opponents to atomistics, it explained many experimental findings about the materials properties of gases, Boyle's law, diffusion and viscosity of gases, laws on heat conductivity, and the law of increasing entropy. Atomistics later provided an important foundation for problems regarding the nature of heat. Physicists such as Hermann von Helmholtz[19] came to believe that atoms govern thermal motion. Tomlinson's paper states early on that "*friction is generally recognized to happen because of interactions between molecules that are very close to each other*" [23]. He theoretically investigated the forces that appear in the relative motion of atoms

16 John Dalton, 1766–1844.
17 Robert Boyle, 1627–1691, United Kingdom.
18 Amedeo Carlo Avogadro, 1776–1856, Italy.
19 Hermann von Helmholtz, 1821–1894, Germany.

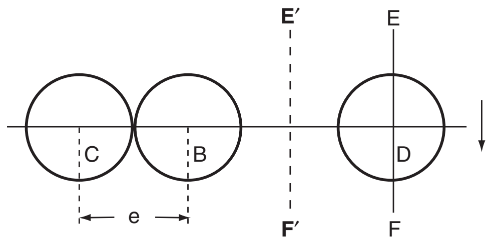

Figure 1.2 Tomlinson's single-pair atom model for explaining energy dissipation in friction [23]. Tomlinson 1929. Reproduced with permission of Taylor and Francis.

in the field of interatomic interactions at the contact surface, and succeeded in rationally explaining the problem of how friction arises from interatomic interactions at the contact surface, or how mechanical energy dissipates into heat energy due to friction, by introducing the concept of ***mechanical adiabaticity***, thereby opening the door to the atomic theory of friction. Figure 1.2 shows the original model in the paper. It has been considered that two solid bodies in contact and with relative sliding motion, and, for simplicity, a single atom D forming part of a body which is moving in the direction of EF past another body, of which B and C form two atoms in the state of equilibrium characteristic of a solid. Let us suppose that the atom D in moving past B along the line EF approaches B to within a distance of the attraction field but outside the range of the repulsion. The passage of D causes a slight disturbance in the position of B, which moves away from C, supposing C to be fixed. The atom D in proceeding further along EF then withdraws from B, which returns to its original position. It is conceivable that B arrives back to its original position with some appreciable velocity and therefore with some added energy, the aggregate of which might correspond to the loss of energy in friction. How does a loss of energy occur in friction? The energy dissipation mechanisms are described in Chapters 2 and 4.

However, very little research on the atomistics of friction followed because of the difficulty in handling the complexity of actual non-well-defined surfaces based on the theory. Friction research has been innovated with recent advances in nanotechnology [5]. Friction research in ideal systems where many factors of friction are identified has been difficult for experimental technology reasons; however, recent measurement technologies, including scanning probe microscopy (SPM) [24–27] and technologies to control very clean well-defined surfaces under ultrahigh vacuum, have enabled direct comparison between theoretical models and experiments [28, 29]. Theory can investigate in detail the fundamental properties of interatomic interactions and the mechanism for the appearance of friction generation using computational experiments on atomistic models [30]. Therefore, ***ideal friction experiments***, where the origin of friction are accurately identified, can be combined with atomic-scale friction simulations, and thus the adequacy of atomic-scale friction theory can now be directly verified. For example, atomic force microscopy (AFM) can accurately measure the friction between the surface of a very sharp tip attached to the end of a cantilever and the surface of a sample using the optical lever method [31], which is a displacement measurement method. The latest experimental devices have enabled the first observations of friction without wear or damage [26]. The adhesion theory cannot be used to investigate such friction without wear, and therefore it was necessary to clarify the origins of friction in terms of atomistics [32].